Figure 1: HIV-1 gp41 Structure and Peptides
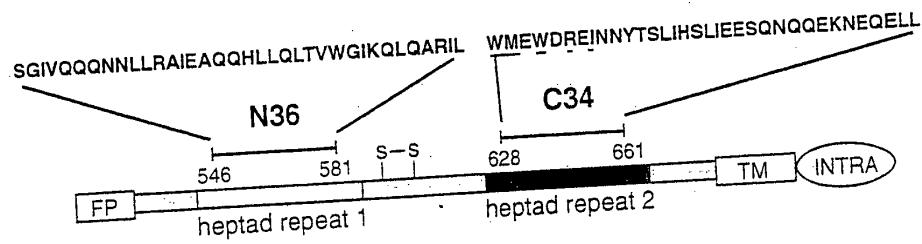

SGIVQQQNNLLRAIEAQQHLLQLTVWGIKQLQARIL

WMEWDREINNYTSLIHSLIEESQNQQEKNEQELL

N36

C34

S–S

546   581   628   661

FP   heptad repeat 1   heptad repeat 2   TM   INTRA

Figure 2: Correlation of C34 Inhibitory Potency With N36/C34 Stability
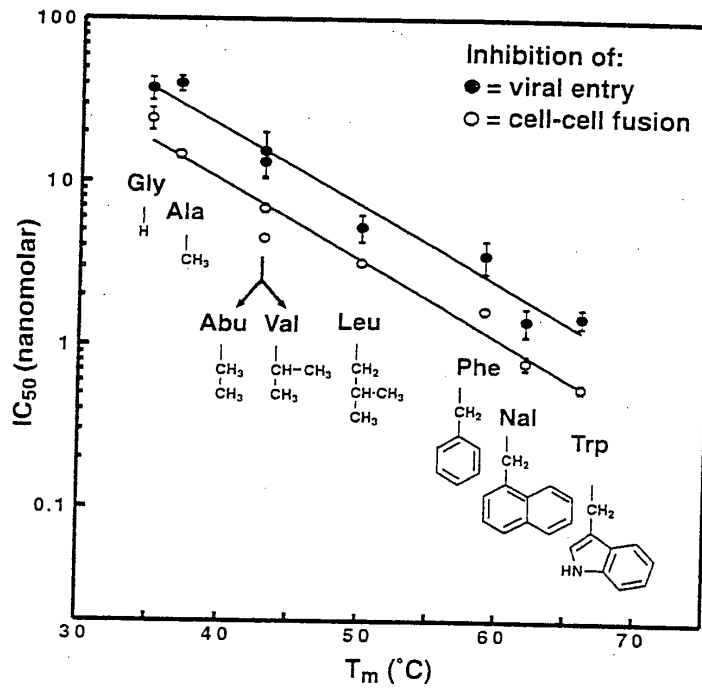
Figure 3: D-peptide Sequences

```
D10pep1 :         Ac- G A C E A R H R E W A W L C A A - CONH2
D10pep1a:    Ac - KK G A C E A R H R E W A W L C A A - CONH2

D10pep3 :    Ac - KK G A C G L G Q E E W F W L C A A - CONH2

D10pep4 :        Ac - G A C D L K A K E W F W L C A A - CONH2

D10pep5 :    Ac - KK G A C E L L G W E W A W L C A A - CONH2
D10pep5a: Ac - KKKK G A C E L L G W E W A W L C A A - CONH2

D10pep6 :        Ac - G A C S R S Q P E W E W L C A A - CONH2
D10pep6a :   Ac - KK G A C S R S Q P E W E W L C A A - CONH2

D10pep7a:    Ac - KK G A C L L R A P E W G W L C A A - CONH2

D10pep10:    Ac - KK G A C M R G E W E W S W L C A A - CONH2

D10pep12:    Ac - K K G A C P P L N K E W A W L C A A - CONH2

Consensus Sequence          C X X X X X E W X W L C
```

Where:
G = glycine
A = alanine
C = cysteine
D = aspartic acid
L = leucine
K = lysine
E = glutamic acid
W = tryptophan
F = phenylalanine
R = arginine
H = histidine
S = serine
Q = glutamine

Figure 4: Mirror-Image Phage Display with the D-IQN17 Target

1. Perform rounds of phage selection to identify binders to D-IQN17.

D-IQN17

Phage Library:
C/SXXXXXXXXXXC/S

←—linker with trypsin site

←—biotin

2. Sequence individual phage clones

3. Test for specificity of binding. Determine if the phage bind to the gp41 region of D-IQN17.

D-IQN17   blank   D-GCN4-pIQI   D-IQN17 (G36W)

X
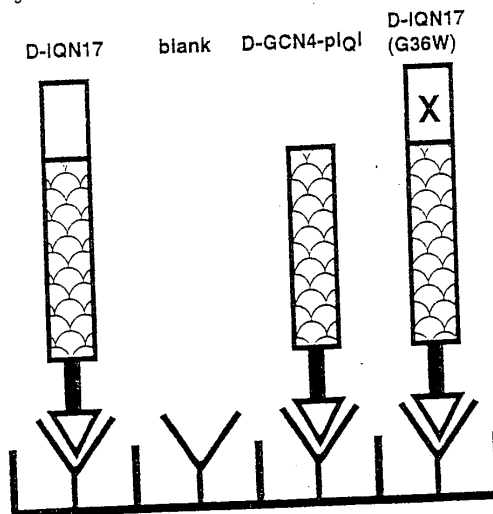
4. Synthesize D-peptides.

5. Assay anti-HIV activity of D-peptides.

Relationship of D-peptides to IQN17

Figure 5A
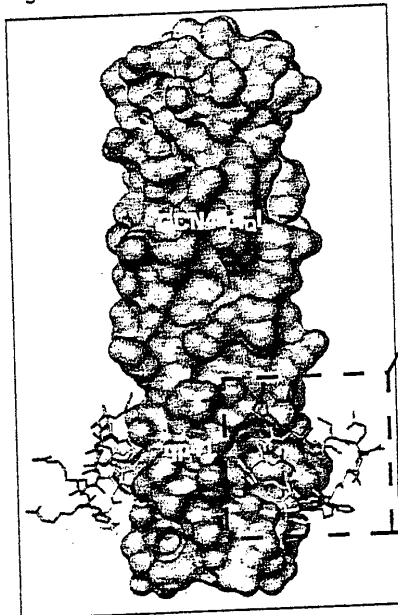
Figure 5B
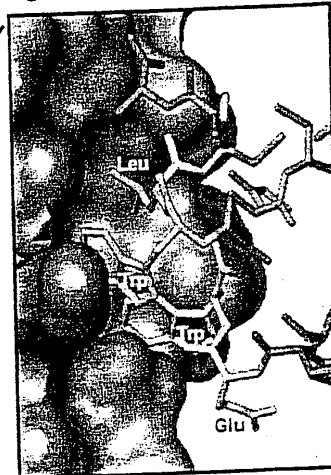
Syncytia Assays

Figure 6A
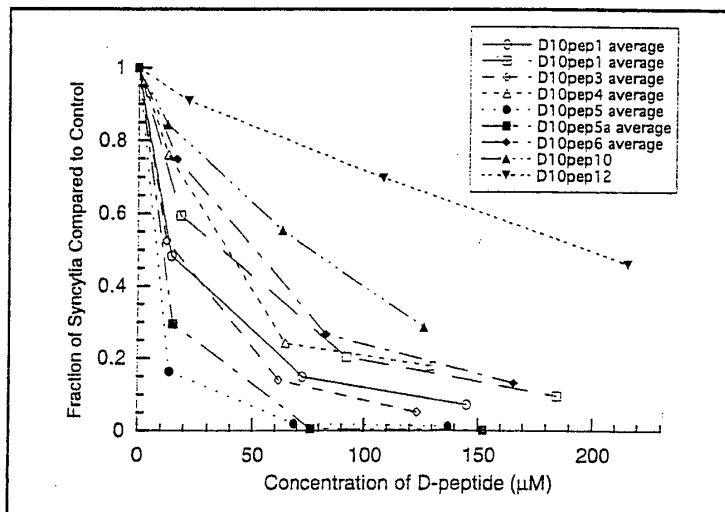
Figure 6B: IC_{50} Data for D-Peptides:

D-Peptide	Approximate IC_{50} Value (from one or more experiments)
D10pep1	2×10^{-5} M
D10pep1A	3×10^{-5} M
D10pep3	1×10^{-5} M
D10pep4	3×10^{-5} M
D10pep5	3×10^{-6} M
D10pep5a	6×10^{-6} M
D10pep6	3×10^{-5} M
D10pep7a	4×10^{-5} M
Dpep10	6×10^{-5} M
Dpep12	2×10^{-4} M

D10pep3
D10pep4   } show anti-viral effects with IC_{50} values of
D10pep5   less than 1×10^{-4} M.

```
REMARK  3
REMARK  3 REFINEMENT.
REMARK  3   PROGRAM       : CNS 0.5
REMARK  3   AUTHORS       : BRUNGER, ADAMS, CLORE, DELANO,
REMARK  3                   GROS, GROSSE-KUNSTLEVE, JIANG,
REMARK  3                   KUSZEWSKI, NILGES, PANNU, READ,
REMARK  3                   RICE, SIMONSON, WARREN
REMARK  3
REMARK  3
REMARK  3   DATA USED IN REFINEMENT.
REMARK  3    RESOLUTION RANGE HIGH (ANGSTROMS) : 1.50
REMARK  3    RESOLUTION RANGE LOW  (ANGSTROMS) :10.00
REMARK  3    DATA CUTOFF            (SIGMA(F)) : 0.0
REMARK  3    DATA CUTOFF HIGH         (ABS(F)) :    646169.44
REMARK  3    DATA CUTOFF LOW          (ABS(F)) :      0.000000
REMARK  3    COMPLETENESS (WORKING+TEST)   (%) : 94.6
REMARK  3    NUMBER OF REFLECTIONS             : 13549
REMARK  3
REMARK  3   FIT TO DATA USED IN REFINEMENT.
REMARK  3    CROSS-VALIDATION METHOD          : THROUGHOUT
REMARK  3    FREE R VALUE TEST SET SELECTION  : RANDOM
REMARK  3    R VALUE            (WORKING SET) : 0.214
REMARK  3    FREE R VALUE                     : 0.245
REMARK  3    FREE R VALUE TEST SET SIZE   (%) : 10.1
REMARK  3    FREE R VALUE TEST SET COUNT      : 1362
REMARK  3    ESTIMATED ERROR OF FREE R VALUE  : 0.007
REMARK  3
REMARK  3   FIT IN THE HIGHEST RESOLUTION BIN.
REMARK  3    TOTAL NUMBER OF BINS USED            :    6
REMARK  3    BIN RESOLUTION RANGE HIGH      (A) : 1.50
REMARK  3    BIN RESOLUTION RANGE LOW       (A) : 1.59
REMARK  3    BIN COMPLETENESS (WORKING+TEST)(%) : 96.1
REMARK  3    REFLECTIONS IN BIN   (WORKING SET) :  2008
REMARK  3    BIN R VALUE          (WORKING SET) : 0.233
REMARK  3    BIN FREE R VALUE                   : 0.270
REMARK  3    BIN FREE R VALUE TEST SET SIZE (%) : 9.8
REMARK  3    BIN FREE R VALUE TEST SET COUNT    :    219
REMARK  3    ESTIMATED ERROR OF BIN FREE R VALUE : 0.018
REMARK  3
REMARK  3   NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.
REMARK  3    PROTEIN ATOMS            :    0
REMARK  3    NUCLEIC ACID ATOMS       :    0
REMARK  3    HETEROGEN ATOMS          :    0
REMARK  3    SOLVENT ATOMS            :    0
REMARK  3
REMARK  3   B VALUES.
REMARK  3    FROM WILSON PLOT          (A**2) : 21.6
REMARK  3    MEAN B VALUE     (OVERALL, A**2) : 29.7
REMARK  3    OVERALL ANISOTROPIC B VALUE.
REMARK  3     B11 (A**2) :  3.61
REMARK  3     B22 (A**2) :  3.61
REMARK  3     B33 (A**2) : -7.22
REMARK  3     B12 (A**2) :  1.74
REMARK  3     B13 (A**2) :  0.00
REMARK  3     B23 (A**2) :  0.00
REMARK  3
REMARK  3   BULK SOLVENT MODELING.
REMARK  3    METHOD USED : FLAT MODEL
REMARK  3    KSOL         : 0.394054
```

Figure 7A

```
REMARK   3  BSOL       : 58.3445 (A**2)
REMARK   3
REMARK   3  ESTIMATED COORDINATE ERROR.
REMARK   3   ESD FROM LUZZATI PLOT         (A) : 0.18
REMARK   3   ESD FROM SIGMAA               (A) : 0.09
REMARK   3   LOW RESOLUTION CUTOFF         (A) : 5.00
REMARK   3
REMARK   3  CROSS-VALIDATED ESTIMATED COORDINATE ERROR.
REMARK   3   ESD FROM C-V LUZZATI PLOT     (A) : 0.20
REMARK   3   ESD FROM C-V SIGMAA           (A) : 0.12
REMARK   3
REMARK   3  RMS DEVIATIONS FROM IDEAL VALUES.
REMARK   3   BOND LENGTHS             (A) : 0.012
REMARK   3   BOND ANGLES        (DEGREES) : 1.5
REMARK   3   DIHEDRAL ANGLES    (DEGREES) : 15.7
REMARK   3   IMPROPER ANGLES    (DEGREES) : 1.00
REMARK   3
REMARK   3  ISOTROPIC THERMAL MODEL : RESTRAINED
REMARK   3
REMARK   3  ISOTROPIC THERMAL FACTOR RESTRAINTS.    RMS     SIGMA
REMARK   3   MAIN-CHAIN BOND      (A**2) : 0.956 ; 2.0
REMARK   3   MAIN-CHAIN ANGLE     (A**2) : 1.503 ; 3.0
REMARK   3   SIDE-CHAIN BOND      (A**2) : 1.853 ; 3.0
REMARK   3   SIDE-CHAIN ANGLE     (A**2) : 2.676 ; 3.5
REMARK   3
REMARK   3  NCS MODEL : NONE
REMARK   3                                       RMS   SIGMA/WEIGHT
REMARK   3  NCS RESTRAINTS.
REMARK   3   GROUP  1  POSITIONAL      (A) : NULL ; NULL
REMARK   3   GROUP  1  B-FACTOR     (A**2) : NULL ; NULL
REMARK   3
REMARK   3  PARAMETER FILE  1  : protein_rep_d.param
REMARK   3  PARAMETER FILE  2  : CNS_TOPPAR/water_rep.param
REMARK   3  PARAMETER FILE  3  : CNS_TOPPAR/ion.param
REMARK   3  TOPOLOGY FILE  1   : CNS_TOPPAR/protein.top
REMARK   3  TOPOLOGY FILE  2   : CNS_TOPPAR/water.top
REMARK   3  TOPOLOGY FILE  3   : CNS_TOPPAR/ion.top
REMARK   3
REMARK   3  OTHER REFINEMENT REMARKS: NULL
SEQRES   1 A  214  ACE ARG MET LYS GLN ILE GLU ASP LYS ILE GLU GLU ILE
SEQRES   2 A  214  GLU SER LYS GLN LYS LYS ILE GLU GLU ILE GLU ILE ALA ARG
SEQRES   3 A  214  ILE LYS LYS LEU LEU GLN LEU THR VAL TRP GLY ILE LYS
SEQRES   4 A  214  GLN LEU GLN ALA ARG ILE LEU ACE DLY DLA DCS DLU DLA
SEQRES   5 A  214  DRG DIS DRG DLU DRP DLA DRP DEU DCS DLA DLA CL WAT
SEQRES   6 A  214  WAT WAT WAT WAT WAT WAT WAT WAT WAT WAT WAT WAT WAT
SEQRES   7 A  214  WAT WAT WAT WAT WAT WAT WAT WAT WAT WAT WAT WAT WAT
SEQRES   8 A  214  WAT WAT WAT WAT WAT WAT WAT WAT WAT WAT WAT WAT WAT
SEQRES   9 A  214  WAT WAT WAT WAT WAT WAT WAT WAT WAT WAT WAT WAT WAT
SEQRES  10 A  214  WAT WAT WAT WAT WAT WAT WAT WAT WAT WAT WAT WAT WAT
SEQRES  11 A  214  WAT WAT WAT WAT WAT WAT WAT WAT WAT WAT WAT WAT WAT
SEQRES  12 A  214  WAT WAT WAT WAT WAT WAT WAT WAT WAT WAT WAT WAT WAT
SEQRES  13 A  214  WAT WAT WAT WAT WAT WAT WAT WAT WAT WAT WAT WAT WAT
SEQRES  14 A  214  WAT WAT WAT WAT WAT WAT WAT WAT WAT WAT WAT WAT WAT
SEQRES  15 A  214  WAT WAT WAT WAT WAT WAT WAT WAT WAT WAT WAT WAT WAT
SEQRES  16 A  214  WAT WAT WAT WAT WAT WAT WAT WAT WAT WAT WAT WAT WAT
SEQRES  17 A  214  WAT WAT WAT WAT WAT WAT
CRYST1   41.829   41.829   84.817  90.00  90.00 120.00 P 3 2 1        6
ORIGX1      1.000000  0.000000  0.000000        0.00000
```

Figure 7B

```
ORIGX2        0.000000  1.000000  0.000000      0.00000
ORIGX3        0.000000  0.000000  1.000000      0.00000
SCALE1        0.023907  0.013803  0.000000      0.00000
SCALE2        0.000000  0.027605  0.000000      0.00000
SCALE3        0.000000  0.000000  0.011790      0.00000
ATOM     1  CA  ACE A   0      26.930   7.813 -22.925  1.00 54.89      A
ATOM     2  C   ACE A   0      26.773   9.004 -22.017  1.00 54.85      A
ATOM     3  O   ACE A   0      25.855   9.820 -22.124  1.00 54.90      A
ATOM     4  N   ARG A   1      27.749   9.121 -21.117  1.00 54.75      A
ATOM     5  CA  ARG A   1      27.815  10.229 -20.165  1.00 54.58      A
ATOM     6  CB  ARG A   1      27.625  11.568 -20.887  1.00 54.54      A
ATOM     7  CG  ARG A   1      27.841  12.790 -20.010  1.00 54.10      A
ATOM     8  CD  ARG A   1      27.657  14.085 -20.800  1.00 54.18      A
ATOM     9  NE  ARG A   1      28.177  15.253 -20.086  1.00 54.02      A
ATOM    10  CZ  ARG A   1      29.470  15.495 -19.870  1.00 54.03      A
ATOM    11  NH1 ARG A   1      30.395  14.654 -20.312  1.00 53.79      A
ATOM    12  NH2 ARG A   1      29.843  16.587 -19.206  1.00 53.77      A
ATOM    13  C   ARG A   1      26.752  10.087 -19.074  1.00 54.54      A
ATOM    14  O   ARG A   1      27.042  10.224 -17.884  1.00 54.51      A
ATOM    15  N   MET A   2      25.518   9.809 -19.480  1.00 54.42      A
ATOM    16  CA  MET A   2      24.445   9.671 -18.515  1.00 54.44      A
ATOM    17  CB  MET A   2      23.074   9.796 -19.202  1.00 54.68      A
ATOM    18  CG  MET A   2      22.749   8.736 -20.238  1.00 54.76      A
ATOM    19  SD  MET A   2      21.345   9.252 -21.275  1.00 55.63      A
ATOM    20  CE  MET A   2      22.189   9.658 -22.822  1.00 55.29      A
ATOM    21  C   MET A   2      24.557   8.360 -17.755  1.00 54.51      A
ATOM    22  O   MET A   2      24.073   8.249 -16.629  1.00 54.42      A
ATOM    23  N   LYS A   3      25.208   7.372 -18.362  1.00 54.34      A
ATOM    24  CA  LYS A   3      25.383   6.082 -17.702  1.00 54.29      A
ATOM    25  CB  LYS A   3      26.212   5.139 -18.581  1.00 54.05      A
ATOM    26  CG  LYS A   3      26.527   3.786 -17.956  1.00 54.04      A
ATOM    27  CD  LYS A   3      27.727   3.853 -17.018  1.00 54.12      A
ATOM    28  CE  LYS A   3      28.108   2.469 -16.513  1.00 54.37      A
ATOM    29  NZ  LYS A   3      29.332   2.493 -15.656  1.00 53.92      A
ATOM    30  C   LYS A   3      26.097   6.344 -16.384  1.00 54.33      A
ATOM    31  O   LYS A   3      25.779   5.740 -15.353  1.00 54.60      A
ATOM    32  N   GLN A   4      27.064   7.255 -16.426  1.00 53.94      A
ATOM    33  CA  GLN A   4      27.811   7.626 -15.236  1.00 53.69      A
ATOM    34  CB  GLN A   4      28.845   8.699 -15.580  1.00 54.21      A
ATOM    35  CG  GLN A   4      29.861   8.974 -14.477  1.00 55.15      A
ATOM    36  CD  GLN A   4      29.621  10.285 -13.732  1.00 55.56      A
ATOM    37  OE1 GLN A   4      29.532  11.354 -14.343  1.00 56.19      A
ATOM    38  NE2 GLN A   4      29.533  10.209 -12.403  1.00 55.66      A
ATOM    39  C   GLN A   4      26.828   8.182 -14.212  1.00 53.19      A
ATOM    40  O   GLN A   4      26.972   7.953 -13.008  1.00 53.10      A
ATOM    41  N   ILE A   5      25.832   8.918 -14.705  1.00 52.58      A
ATOM    42  CA  ILE A   5      24.817   9.523 -13.853  1.00 51.70      A
ATOM    43  CB  ILE A   5      23.826  10.380 -14.687  1.00 51.71      A
ATOM    44  CG2 ILE A   5      22.643  10.812 -13.831  1.00 51.41      A
ATOM    45  CG1 ILE A   5      24.547  11.611 -15.246  1.00 51.48      A
ATOM    46  CD1 ILE A   5      23.646  12.569 -16.017  1.00 51.33      A
ATOM    47  C   ILE A   5      24.051   8.467 -13.060  1.00 51.26      A
ATOM    48  O   ILE A   5      23.650   8.700 -11.920  1.00 51.09      A
ATOM    49  N   GLU A   6      23.864   7.300 -13.662  1.00 50.54      A
ATOM    50  CA  GLU A   6      23.146   6.214 -13.013  1.00 50.01      A
ATOM    51  CB  GLU A   6      22.789   5.148 -14.043  1.00 50.43      A
ATOM    52  CG  GLU A   6      22.141   5.721 -15.289  1.00 51.26      A
ATOM    53  CD  GLU A   6      22.045   4.703 -16.400  1.00 51.68      A
```

Figure 7C

ATOM	54	OE1	GLU	A	6	23.016	3.931	-16.557	1.00	52.29	A
ATOM	55	OE2	GLU	A	6	21.019	4.682	-17.116	1.00	52.25	A
ATOM	56	C	GLU	A	6	23.995	5.606	-11.904	1.00	49.32	A
ATOM	57	O	GLU	A	6	23.475	5.210	-10.859	1.00	49.24	A
ATOM	58	N	ASP	A	7	25.302	5.527	-12.128	1.00	48.32	A
ATOM	59	CA	ASP	A	7	26.178	4.970	-11.113	1.00	47.23	A
ATOM	60	CB	ASP	A	7	27.543	4.626	-11.703	1.00	47.92	A
ATOM	61	CG	ASP	A	7	27.450	3.585	-12.788	1.00	48.33	A
ATOM	62	OD1	ASP	A	7	26.526	2.741	-12.729	1.00	48.43	A
ATOM	63	OD2	ASP	A	7	28.310	3.606	-13.690	1.00	48.94	A
ATOM	64	C	ASP	A	7	26.344	5.920	-9.926	1.00	46.09	A
ATOM	65	O	ASP	A	7	26.283	5.481	-8.773	1.00	45.71	A
ATOM	66	N	LYS	A	8	26.551	7.209	-10.201	1.00	44.57	A
ATOM	67	CA	LYS	A	8	26.703	8.195	-9.129	1.00	43.01	A
ATOM	68	CB	LYS	A	8	26.959	9.598	-9.708	1.00	43.49	A
ATOM	69	CG	LYS	A	8	25.895	10.076	-10.695	1.00	44.78	A
ATOM	70	CD	LYS	A	8	26.423	11.125	-11.702	1.00	45.38	A
ATOM	71	CE	LYS	A	8	26.698	12.490	-11.068	1.00	45.64	A
ATOM	72	NZ	LYS	A	8	27.153	13.499	-12.069	1.00	45.55	A
ATOM	73	C	LYS	A	8	25.413	8.171	-8.318	1.00	41.20	A
ATOM	74	O	LYS	A	8	25.419	8.346	-7.098	1.00	40.61	A
ATOM	75	N	ILE	A	9	24.302	7.935	-9.002	1.00	39.40	A
ATOM	76	CA	ILE	A	9	23.015	7.859	-8.333	1.00	37.29	A
ATOM	77	CB	ILE	A	9	21.872	7.859	-9.358	1.00	37.14	A
ATOM	78	CG2	ILE	A	9	20.600	7.251	-8.759	1.00	37.06	A
ATOM	79	CG1	ILE	A	9	21.631	9.303	-9.812	1.00	36.95	A
ATOM	80	CD1	ILE	A	9	20.801	9.440	-11.066	1.00	36.89	A
ATOM	81	C	ILE	A	9	22.927	6.638	-7.418	1.00	36.07	A
ATOM	82	O	ILE	A	9	22.450	6.756	-6.292	1.00	34.70	A
ATOM	83	N	GLU	A	10	23.389	5.478	-7.887	1.00	34.23	A
ATOM	84	CA	GLU	A	10	23.353	4.260	-7.074	1.00	33.04	A
ATOM	85	CB	GLU	A	10	23.884	3.013	-7.847	1.00	32.87	A
ATOM	86	CG	GLU	A	10	23.890	1.705	-6.991	1.00	33.10	A
ATOM	87	CD	GLU	A	10	24.287	0.417	-7.747	1.00	33.56	A
ATOM	88	OE1	GLU	A	10	24.327	0.442	-8.999	1.00	34.07	A
ATOM	89	OE2	GLU	A	10	24.542	-0.630	-7.084	1.00	32.41	A
ATOM	90	C	GLU	A	10	24.244	4.556	-5.878	1.00	32.53	A
ATOM	91	O	GLU	A	10	24.009	4.069	-4.779	1.00	32.14	A
ATOM	92	N	GLU	A	11	25.259	5.380	-6.100	1.00	31.82	A
ATOM	93	CA	GLU	A	11	26.165	5.731	-5.018	1.00	31.36	A
ATOM	94	CB	GLU	A	11	27.409	6.445	-5.536	1.00	33.18	A
ATOM	95	CG	GLU	A	11	28.358	6.833	-4.423	1.00	35.22	A
ATOM	96	CD	GLU	A	11	29.105	5.643	-3.822	1.00	36.93	A
ATOM	97	OE1	GLU	A	11	28.488	4.580	-3.575	1.00	38.03	A
ATOM	98	OE2	GLU	A	11	30.322	5.774	-3.579	1.00	38.85	A
ATOM	99	C	GLU	A	11	25.456	6.621	-3.998	1.00	30.15	A
ATOM	100	O	GLU	A	11	25.556	6.377	-2.798	1.00	28.89	A
ATOM	101	N	ILE	A	12	24.737	7.640	-4.471	1.00	29.09	A
ATOM	102	CA	ILE	A	12	24.017	8.533	-3.550	1.00	28.34	A
ATOM	103	CB	ILE	A	12	23.301	9.675	-4.325	1.00	28.74	A
ATOM	104	CG2	ILE	A	12	22.206	10.281	-3.501	1.00	28.70	A
ATOM	105	CG1	ILE	A	12	24.327	10.743	-4.701	1.00	28.84	A
ATOM	106	CD1	ILE	A	12	23.922	11.603	-5.890	1.00	29.69	A
ATOM	107	C	ILE	A	12	22.985	7.725	-2.761	1.00	27.83	A
ATOM	108	O	ILE	A	12	22.802	7.948	-1.560	1.00	26.46	A
ATOM	109	N	GLU	A	13	22.312	6.790	-3.423	1.00	27.40	A
ATOM	110	CA	GLU	A	13	21.313	5.965	-2.762	1.00	26.92	A
ATOM	111	CB	GLU	A	13	20.579	5.087	-3.805	1.00	28.34	A

Figure 7D

ATOM	112	CG	GLU	A	13	19.760	5.927	-4.810	1.00	29.72	A
ATOM	113	CD	GLU	A	13	19.080	5.118	-5.900	1.00	31.77	A
ATOM	114	OE1	GLU	A	13	19.671	4.107	-6.331	1.00	33.64	A
ATOM	115	OE2	GLU	A	13	17.960	5.495	-6.327	1.00	32.24	A
ATOM	116	C	GLU	A	13	21.975	5.110	-1.678	1.00	26.36	A
ATOM	117	O	GLU	A	13	21.411	4.912	-0.597	1.00	25.75	A
ATOM	118	N	SER	A	14	23.179	4.629	-1.950	1.00	26.17	A
ATOM	119	CA	SER	A	14	23.899	3.792	-0.999	1.00	26.31	A
ATOM	120	CB	SER	A	14	25.184	3.224	-1.625	1.00	26.71	A
ATOM	121	OG	SER	A	14	25.954	2.470	-0.695	1.00	30.07	A
ATOM	122	C	SER	A	14	24.246	4.626	0.221	1.00	25.81	A
ATOM	123	O	SER	A	14	24.079	4.149	1.339	1.00	25.13	A
ATOM	124	N	LYS	A	15	24.753	5.840	0.009	1.00	24.70	A
ATOM	125	CA	LYS	A	15	25.091	6.713	1.151	1.00	25.41	A
ATOM	126	CB	LYS	A	15	25.805	7.971	0.672	1.00	26.20	A
ATOM	127	CG	LYS	A	15	27.256	7.762	0.285	1.00	29.07	A
ATOM	128	CD	LYS	A	15	27.875	9.077	-0.220	1.00	30.97	A
ATOM	129	CE	LYS	A	15	29.328	8.914	-0.603	1.00	32.08	A
ATOM	130	NZ	LYS	A	15	29.547	7.749	-1.502	1.00	34.63	A
ATOM	131	C	LYS	A	15	23.824	7.102	1.938	1.00	24.45	A
ATOM	132	O	LYS	A	15	23.862	7.279	3.171	1.00	24.50	A
ATOM	133	N	GLN	A	16	22.708	7.254	1.247	1.00	24.12	A
ATOM	134	CA	GLN	A	16	21.450	7.586	1.904	1.00	23.82	A
ATOM	135	CB	GLN	A	16	20.396	7.815	0.834	1.00	25.71	A
ATOM	136	CG	GLN	A	16	19.229	8.643	1.232	1.00	29.64	A
ATOM	137	CD	GLN	A	16	18.543	9.230	0.004	1.00	32.26	A
ATOM	138	OE1	GLN	A	16	18.015	8.498	-0.817	1.00	34.89	A
ATOM	139	NE2	GLN	A	16	18.569	10.556	-0.135	1.00	32.74	A
ATOM	140	C	GLN	A	16	21.027	6.447	2.838	1.00	23.67	A
ATOM	141	O	GLN	A	16	20.584	6.681	3.979	1.00	22.84	A
ATOM	142	N	LYS	A	17	21.160	5.214	2.365	1.00	22.83	A
ATOM	143	CA	LYS	A	17	20.798	4.057	3.179	1.00	22.59	A
ATOM	144	CB	LYS	A	17	20.939	2.756	2.357	1.00	22.86	A
ATOM	145	CG	LYS	A	17	20.340	1.539	3.055	1.00	26.69	A
ATOM	146	CD	LYS	A	17	18.837	1.579	2.932	1.00	29.27	A
ATOM	147	CE	LYS	A	17	18.177	0.837	4.051	1.00	31.75	A
ATOM	148	NZ	LYS	A	17	16.686	0.870	3.940	1.00	34.25	A
ATOM	149	C	LYS	A	17	21.718	4.015	4.406	1.00	22.31	A
ATOM	150	O	LYS	A	17	21.261	3.747	5.515	1.00	21.02	A
ATOM	151	N	LYS	A	18	23.001	4.306	4.223	1.00	21.81	A
ATOM	152	CA	LYS	A	18	23.909	4.302	5.374	1.00	21.74	A
ATOM	153	CB	LYS	A	18	25.348	4.540	4.964	1.00	24.04	A
ATOM	154	CG	LYS	A	18	26.029	3.321	4.401	1.00	27.30	A
ATOM	155	CD	LYS	A	18	27.381	3.712	3.863	1.00	29.23	A
ATOM	156	CE	LYS	A	18	27.972	2.592	3.025	1.00	30.50	A
ATOM	157	NZ	LYS	A	18	29.290	3.010	2.472	1.00	33.57	A
ATOM	158	C	LYS	A	18	23.500	5.376	6.378	1.00	20.62	A
ATOM	159	O	LYS	A	18	23.565	5.138	7.577	1.00	19.85	A
ATOM	160	N	ILE	A	19	23.062	6.531	5.887	1.00	19.99	A
ATOM	161	CA	ILE	A	19	22.655	7.636	6.762	1.00	19.98	A
ATOM	162	CB	ILE	A	19	22.406	8.926	5.914	1.00	20.09	A
ATOM	163	CG2	ILE	A	19	21.554	9.944	6.682	1.00	20.80	A
ATOM	164	CG1	ILE	A	19	23.756	9.499	5.464	1.00	21.49	A
ATOM	165	CD1	ILE	A	19	23.669	10.495	4.296	1.00	21.18	A
ATOM	166	C	ILE	A	19	21.400	7.221	7.517	1.00	20.44	A
ATOM	167	O	ILE	A	19	21.282	7.452	8.735	1.00	20.23	A
ATOM	168	N	GLU	A	20	20.459	6.569	6.836	1.00	20.24	A
ATOM	169	CA	GLU	A	20	19.230	6.149	7.503	1.00	20.43	A

Figure 7E

ATOM	170	CB	GLU	A	20	18.223	5.608	6.484	1.00	22.94	A
ATOM	171	CG	GLU	A	20	17.766	6.671	5.499	1.00	25.51	A
ATOM	172	CD	GLU	A	20	16.926	6.108	4.378	1.00	29.04	A
ATOM	173	OE1	GLU	A	20	16.961	4.873	4.177	1.00	30.40	A
ATOM	174	OE2	GLU	A	20	16.243	6.901	3.691	1.00	30.73	A
ATOM	175	C	GLU	A	20	19.533	5.109	8.576	1.00	20.88	A
ATOM	176	O	GLU	A	20	18.917	5.127	9.645	1.00	20.23	A
ATOM	177	N	ASN	A	21	20.478	4.220	8.321	1.00	20.53	A
ATOM	178	CA	ASN	A	21	20.820	3.212	9.328	1.00	21.87	A
ATOM	179	CB	ASN	A	21	21.694	2.117	8.720	1.00	24.15	A
ATOM	180	CG	ASN	A	21	20.875	1.155	7.872	1.00	25.28	A
ATOM	181	OD1	ASN	A	21	19.676	0.980	8.099	1.00	28.26	A
ATOM	182	ND2	ASN	A	21	21.505	0.549	6.870	1.00	26.78	A
ATOM	183	C	ASN	A	21	21.500	3.854	10.527	1.00	21.75	A
ATOM	184	O	ASN	A	21	21.269	3.444	11.674	1.00	21.80	A
ATOM	185	N	GLU	A	22	22.335	4.853	10.274	1.00	20.99	A
ATOM	186	CA	GLU	A	22	23.007	5.548	11.369	1.00	20.36	A
ATOM	187	CB	GLU	A	22	24.059	6.516	10.825	1.00	22.89	A
ATOM	188	CG	GLU	A	22	24.914	7.169	11.901	1.00	25.86	A
ATOM	189	CD	GLU	A	22	25.515	6.170	12.882	1.00	27.97	A
ATOM	190	OE1	GLU	A	22	26.121	5.158	12.444	1.00	30.05	A
ATOM	191	OE2	GLU	A	22	25.376	6.411	14.118	1.00	31.29	A
ATOM	192	C	GLU	A	22	21.952	6.294	12.187	1.00	19.79	A
ATOM	193	O	GLU	A	22	21.988	6.264	13.445	1.00	18.87	A
ATOM	194	N	ILE	A	23	21.003	6.951	11.518	1.00	18.92	A
ATOM	195	CA	ILE	A	23	19.955	7.670	12.254	1.00	18.60	A
ATOM	196	CB	ILE	A	23	19.012	8.388	11.244	1.00	18.79	A
ATOM	197	CG2	ILE	A	23	17.672	8.764	11.880	1.00	20.11	A
ATOM	198	CG1	ILE	A	23	19.739	9.598	10.701	1.00	20.45	A
ATOM	199	CD1	ILE	A	23	19.060	10.223	9.539	1.00	22.51	A
ATOM	200	C	ILE	A	23	19.163	6.687	13.118	1.00	19.09	A
ATOM	201	O	ILE	A	23	18.807	7.006	14.260	1.00	18.74	A
ATOM	202	N	ALA	A	24	18.903	5.479	12.617	1.00	18.44	A
ATOM	203	CA	ALA	A	24	18.153	4.517	13.420	1.00	18.86	A
ATOM	204	CB	ALA	A	24	17.824	3.257	12.573	1.00	19.39	A
ATOM	205	C	ALA	A	24	18.947	4.136	14.665	1.00	18.66	A
ATOM	206	O	ALA	A	24	18.343	3.966	15.757	1.00	19.32	A
ATOM	207	N	ARG	A	25	20.272	4.028	14.548	1.00	18.57	A
ATOM	208	CA	ARG	A	25	21.111	3.667	15.709	1.00	19.19	A
ATOM	209	CB	ARG	A	25	22.552	3.343	15.287	1.00	20.85	A
ATOM	210	CG	ARG	A	25	22.674	1.959	14.627	1.00	23.87	A
ATOM	211	CD	ARG	A	25	24.108	1.536	14.429	1.00	25.32	A
ATOM	212	NE	ARG	A	25	24.759	2.294	13.376	1.00	27.13	A
ATOM	213	CZ	ARG	A	25	24.672	2.019	12.075	1.00	27.60	A
ATOM	214	NH1	ARG	A	25	23.955	0.979	11.641	1.00	29.92	A
ATOM	215	NH2	ARG	A	25	25.296	2.806	11.214	1.00	27.79	A
ATOM	216	C	ARG	A	25	21.083	4.819	16.722	1.00	18.69	A
ATOM	217	O	ARG	A	25	20.942	4.592	17.940	1.00	17.93	A
ATOM	218	N	ILE	A	26	21.201	6.041	16.221	1.00	17.83	A
ATOM	219	CA	ILE	A	26	21.184	7.222	17.080	1.00	16.94	A
ATOM	220	CB	ILE	A	26	21.369	8.479	16.225	1.00	17.99	A
ATOM	221	CG2	ILE	A	26	20.943	9.741	17.006	1.00	19.34	A
ATOM	222	CG1	ILE	A	26	22.821	8.537	15.796	1.00	19.88	A
ATOM	223	CD1	ILE	A	26	23.144	9.587	14.721	1.00	21.83	A
ATOM	224	C	ILE	A	26	19.876	7.301	17.857	1.00	18.02	A
ATOM	225	O	ILE	A	26	19.875	7.580	19.055	1.00	17.73	A
ATOM	226	N	LYS	A	27	18.752	7.069	17.191	1.00	17.60	A
ATOM	227	CA	LYS	A	27	17.450	7.137	17.853	1.00	17.90	A

Figure 7F

ATOM	228	CB	LYS A	27	16.330	6.994	16.805	1.00	19.01	A
ATOM	229	CG	LYS A	27	16.266	8.210	15.876	1.00	22.27	A
ATOM	230	CD	LYS A	27	15.275	7.984	14.711	1.00	24.03	A
ATOM	231	CE	LYS A	27	13.860	7.664	15.161	1.00	24.41	A
ATOM	232	NZ	LYS A	27	13.173	8.848	15.714	1.00	27.04	A
ATOM	233	C	LYS A	27	17.326	6.097	18.969	1.00	18.17	A
ATOM	234	O	LYS A	27	16.767	6.388	20.013	1.00	18.33	A
ATOM	235	N	LYS A	28	17.871	4.896	18.775	1.00	17.00	A
ATOM	236	CA	LYS A	28	17.788	3.867	19.790	1.00	17.21	A
ATOM	237	CB	LYS A	28	18.244	2.503	19.223	1.00	18.92	A
ATOM	238	CG	LYS A	28	17.288	1.982	18.164	1.00	24.56	A
ATOM	239	CD	LYS A	28	17.833	0.732	17.464	1.00	26.88	A
ATOM	240	CE	LYS A	28	16.950	0.371	16.260	1.00	28.84	A
ATOM	241	NZ	LYS A	28	17.284	-0.938	15.592	1.00	31.36	A
ATOM	242	C	LYS A	28	18.618	4.257	21.016	1.00	17.36	A
ATOM	243	O	LYS A	28	18.169	4.066	22.165	1.00	17.54	A
ATOM	244	N	LEU A	29	19.794	4.835	20.793	1.00	16.84	A
ATOM	245	CA	LEU A	29	20.642	5.234	21.912	1.00	16.41	A
ATOM	246	CB	LEU A	29	22.077	5.529	21.453	1.00	16.26	A
ATOM	247	CG	LEU A	29	23.050	6.048	22.515	1.00	16.76	A
ATOM	248	CD1	LEU A	29	23.062	5.096	23.701	1.00	16.47	A
ATOM	249	CD2	LEU A	29	24.450	6.201	21.885	1.00	17.67	A
ATOM	250	C	LEU A	29	20.023	6.429	22.606	1.00	16.92	A
ATOM	251	O	LEU A	29	20.027	6.503	23.859	1.00	16.36	A
ATOM	252	N	LEU A	30	19.447	7.343	21.820	1.00	15.57	A
ATOM	253	CA	LEU A	30	18.818	8.519	22.424	1.00	15.77	A
ATOM	254	CB	LEU A	30	18.401	9.501	21.298	1.00	15.65	A
ATOM	255	CG	LEU A	30	17.717	10.780	21.696	1.00	17.55	A
ATOM	256	CD1	LEU A	30	18.557	11.504	22.722	1.00	16.71	A
ATOM	257	CD2	LEU A	30	17.552	11.602	20.399	1.00	18.10	A
ATOM	258	C	LEU A	30	17.659	8.067	23.288	1.00	16.42	A
ATOM	259	O	LEU A	30	17.466	8.604	24.399	1.00	17.55	A
ATOM	260	N	GLN A	31	16.903	7.053	22.862	1.00	16.79	A
ATOM	261	CA	GLN A	31	15.816	6.564	23.692	1.00	18.13	A
ATOM	262	CB	GLN A	31	14.945	5.593	22.886	1.00	21.45	A
ATOM	263	CG	GLN A	31	14.119	6.358	21.834	1.00	24.92	A
ATOM	264	CD	GLN A	31	13.196	7.437	22.424	1.00	26.81	A
ATOM	265	OE1	GLN A	31	12.913	8.459	21.786	1.00	28.75	A
ATOM	266	NE2	GLN A	31	12.713	7.207	23.648	1.00	29.86	A
ATOM	267	C	GLN A	31	16.319	5.958	25.008	1.00	17.24	A
ATOM	268	O	GLN A	31	15.655	6.092	26.038	1.00	17.79	A
ATOM	269	N	LEU A	32	17.494	5.307	24.987	1.00	15.77	A
ATOM	270	CA	LEU A	32	18.070	4.755	26.209	1.00	14.63	A
ATOM	271	CB	LEU A	32	19.314	3.932	25.911	1.00	16.13	A
ATOM	272	CG	LEU A	32	19.015	2.574	25.275	1.00	18.58	A
ATOM	273	CD1	LEU A	32	20.291	1.961	24.770	1.00	20.70	A
ATOM	274	CD2	LEU A	32	18.337	1.698	26.315	1.00	22.17	A
ATOM	275	C	LEU A	32	18.449	5.895	27.140	1.00	13.68	A
ATOM	276	O	LEU A	32	18.258	5.774	28.357	1.00	13.31	A
ATOM	277	N	THR A	33	18.980	6.991	26.600	1.00	13.42	A
ATOM	278	CA	THR A	33	19.348	8.081	27.500	1.00	12.96	A
ATOM	279	CB	THR A	33	20.236	9.134	26.820	1.00	13.48	A
ATOM	280	OG1	THR A	33	19.530	9.745	25.733	1.00	15.60	A
ATOM	281	CG2	THR A	33	21.567	8.508	26.358	1.00	15.01	A
ATOM	282	C	THR A	33	18.124	8.742	28.117	1.00	13.65	A
ATOM	283	O	THR A	33	18.159	9.169	29.285	1.00	12.67	A
ATOM	284	N	VAL A	34	17.038	8.838	27.345	1.00	13.20	A
ATOM	285	CA	VAL A	34	15.804	9.410	27.863	1.00	13.88	A

Figure 7G

ATOM	286	CB	VAL	A	34	14.708	9.498	26.773	1.00	14.31	A
ATOM	287	CG1	VAL	A	34	13.380	9.811	27.382	1.00	15.35	A
ATOM	288	CG2	VAL	A	34	15.096	10.517	25.710	1.00	15.04	A
ATOM	289	C	VAL	A	34	15.326	8.526	29.041	1.00	12.55	A
ATOM	290	O	VAL	A	34	14.997	9.016	30.131	1.00	13.43	A
ATOM	291	N	TRP	A	35	15.354	7.210	28.857	1.00	13.04	A
ATOM	292	CA	TRP	A	35	14.946	6.289	29.908	1.00	13.11	A
ATOM	293	CB	TRP	A	35	14.988	4.861	29.319	1.00	14.19	A
ATOM	294	CG	TRP	A	35	14.672	3.785	30.334	1.00	15.43	A
ATOM	295	CD2	TRP	A	35	15.610	3.101	31.191	1.00	15.26	A
ATOM	296	CE2	TRP	A	35	14.860	2.165	31.963	1.00	15.57	A
ATOM	297	CE3	TRP	A	35	16.990	3.196	31.393	1.00	15.49	A
ATOM	298	CD1	TRP	A	35	13.454	3.258	30.609	1.00	17.15	A
ATOM	299	NE1	TRP	A	35	13.553	2.281	31.572	1.00	17.80	A
ATOM	300	CZ2	TRP	A	35	15.459	1.324	32.905	1.00	15.31	A
ATOM	301	CZ3	TRP	A	35	17.600	2.355	32.349	1.00	16.17	A
ATOM	302	CH2	TRP	A	35	16.815	1.437	33.090	1.00	14.74	A
ATOM	303	C	TRP	A	35	15.869	6.429	31.141	1.00	13.13	A
ATOM	304	O	TRP	A	35	15.418	6.409	32.278	1.00	12.76	A
ATOM	305	N	GLY	A	36	17.176	6.556	30.893	1.00	12.50	A
ATOM	306	CA	GLY	A	36	18.118	6.668	31.998	1.00	12.50	A
ATOM	307	C	GLY	A	36	17.887	7.936	32.817	1.00	11.58	A
ATOM	308	O	GLY	A	36	17.917	7.875	34.042	1.00	11.70	A
ATOM	309	N	ILE	A	37	17.656	9.084	32.174	1.00	11.85	A
ATOM	310	CA	ILE	A	37	17.383	10.303	32.884	1.00	11.18	A
ATOM	311	CB	ILE	A	37	17.262	11.439	31.882	1.00	11.22	A
ATOM	312	CG2	ILE	A	37	16.680	12.660	32.600	1.00	13.25	A
ATOM	313	CG1	ILE	A	37	18.636	11.739	31.281	1.00	12.70	A
ATOM	314	CD1	ILE	A	37	18.571	12.560	29.955	1.00	13.00	A
ATOM	315	C	ILE	A	37	16.082	10.105	33.703	1.00	11.99	A
ATOM	316	O	ILE	A	37	16.026	10.526	34.860	1.00	12.24	A
ATOM	317	N	LYS	A	38	15.069	9.465	33.094	1.00	11.84	A
ATOM	318	CA	LYS	A	38	13.825	9.215	33.809	1.00	13.62	A
ATOM	319	CB	LYS	A	38	12.840	8.512	32.861	1.00	15.00	A
ATOM	320	CG	LYS	A	38	11.429	8.437	33.369	1.00	17.76	A
ATOM	321	CD	LYS	A	38	10.545	7.835	32.247	1.00	20.78	A
ATOM	322	CE	LYS	A	38	9.046	7.955	32.600	1.00	25.34	A
ATOM	323	NZ	LYS	A	38	8.721	7.069	33.722	1.00	29.03	A
ATOM	324	C	LYS	A	38	14.060	8.399	35.083	1.00	12.64	A
ATOM	325	O	LYS	A	38	13.490	8.724	36.163	1.00	12.58	A
ATOM	326	N	GLN	A	39	14.916	7.371	35.001	1.00	11.99	A
ATOM	327	CA	GLN	A	39	15.176	6.573	36.189	1.00	11.84	A
ATOM	328	CB	GLN	A	39	16.049	5.339	35.900	1.00	12.90	A
ATOM	329	CG	GLN	A	39	15.580	4.440	34.757	1.00	14.71	A
ATOM	330	CD	GLN	A	39	14.118	4.213	34.747	1.00	17.73	A
ATOM	331	OE1	GLN	A	39	13.596	3.581	35.669	1.00	22.45	A
ATOM	332	NE2	GLN	A	39	13.420	4.701	33.701	1.00	20.02	A
ATOM	333	C	GLN	A	39	15.907	7.372	37.259	1.00	12.24	A
ATOM	334	O	GLN	A	39	15.601	7.271	38.453	1.00	12.42	A
ATOM	335	N	LEU	A	40	16.883	8.195	36.854	1.00	10.89	A
ATOM	336	CA	LEU	A	40	17.632	8.980	37.853	1.00	11.44	A
ATOM	337	CB	LEU	A	40	18.860	9.648	37.198	1.00	12.26	A
ATOM	338	CG	LEU	A	40	19.827	8.591	36.635	1.00	12.85	A
ATOM	339	CD1	LEU	A	40	21.007	9.367	36.066	1.00	16.06	A
ATOM	340	CD2	LEU	A	40	20.293	7.526	37.650	1.00	17.91	A
ATOM	341	C	LEU	A	40	16.763	10.046	38.497	1.00	10.71	A
ATOM	342	O	LEU	A	40	16.848	10.258	39.701	1.00	11.30	A
ATOM	343	N	GLN	A	41	15.911	10.692	37.704	1.00	11.62	A

Figure 7H

ATOM	344	CA	GLN	A	41	15.038	11.695	38.322	1.00	11.12	A
ATOM	345	CB	GLN	A	41	14.241	12.447	37.257	1.00	11.92	A
ATOM	346	CG	GLN	A	41	13.250	13.381	37.845	1.00	11.53	A
ATOM	347	CD	GLN	A	41	12.280	13.933	36.838	1.00	12.64	A
ATOM	348	OE1	GLN	A	41	11.814	13.226	35.962	1.00	13.16	A
ATOM	349	NE2	GLN	A	41	11.972	15.220	36.973	1.00	13.67	A
ATOM	350	C	GLN	A	41	14.081	11.031	39.332	1.00	10.98	A
ATOM	351	O	GLN	A	41	13.883	11.585	40.404	1.00	12.39	A
ATOM	352	N	ALA	A	42	13.571	9.845	38.994	1.00	12.53	A
ATOM	353	CA	ALA	A	42	12.642	9.185	39.928	1.00	12.08	A
ATOM	354	CB	ALA	A	42	12.035	7.954	39.295	1.00	13.83	A
ATOM	355	C	ALA	A	42	13.383	8.856	41.218	1.00	14.57	A
ATOM	356	O	ALA	A	42	12.820	8.975	42.296	1.00	15.73	A
ATOM	357	N	ARG	A	43	14.647	8.446	41.147	1.00	13.64	A
ATOM	358	CA	ARG	A	43	15.412	8.150	42.327	1.00	16.22	A
ATOM	359	CB	ARG	A	43	16.772	7.626	41.852	1.00	18.06	A
ATOM	360	CG	ARG	A	43	17.706	7.309	42.895	1.00	22.64	A
ATOM	361	CD	ARG	A	43	17.232	6.108	43.679	1.00	25.20	A
ATOM	362	NE	ARG	A	43	18.302	5.922	44.577	1.00	27.65	A
ATOM	363	CZ	ARG	A	43	18.943	4.798	44.758	1.00	20.75	A
ATOM	364	NH1	ARG	A	43	18.607	3.666	44.107	1.00	24.75	A
ATOM	365	NH2	ARG	A	43	19.983	4.899	45.516	1.00	23.93	A
ATOM	366	C	ARG	A	43	15.606	9.411	43.196	1.00	15.07	A
ATOM	367	O	ARG	A	43	15.441	9.372	44.435	1.00	17.46	A
ATOM	368	N	ILE	A	44	15.930	10.529	42.553	1.00	14.44	A
ATOM	369	CA	ILE	A	44	16.181	11.794	43.242	1.00	14.63	A
ATOM	370	CB	ILE	A	44	16.801	12.854	42.280	1.00	15.70	A
ATOM	371	CG2	ILE	A	44	16.817	14.226	42.941	1.00	16.89	A
ATOM	372	CG1	ILE	A	44	18.236	12.422	41.940	1.00	16.08	A
ATOM	373	CD1	ILE	A	44	18.765	13.127	40.739	1.00	19.48	A
ATOM	374	C	ILE	A	44	14.906	12.326	43.887	1.00	16.35	A
ATOM	375	O	ILE	A	44	14.984	12.862	44.991	1.00	19.28	A
ATOM	376	N	LEU	A	45	13.747	12.150	43.258	1.00	15.72	A
ATOM	377	CA	LEU	A	45	12.515	12.682	43.883	1.00	15.80	A
ATOM	378	CB	LEU	A	45	11.505	13.032	42.801	1.00	15.66	A
ATOM	379	CG	LEU	A	45	11.867	14.181	41.878	1.00	15.35	A
ATOM	380	CD1	LEU	A	45	10.793	14.298	40.823	1.00	17.27	A
ATOM	381	CD2	LEU	A	45	11.954	15.485	42.701	1.00	18.49	A
ATOM	382	C	LEU	A	45	11.903	11.710	44.867	1.00	18.22	A
ATOM	383	O	LEU	A	45	11.053	12.187	45.658	1.00	19.14	A
ATOM	384	NT	LEU	A	45	12.258	10.488	44.884	1.00	20.39	A
ATOM	385	CA	ACE	D	0	10.275	-0.794	28.942	1.00	41.14	B
ATOM	386	C	ACE	D	0	11.674	-0.285	28.785	1.00	40.52	B
ATOM	387	O	ACE	D	0	11.905	0.677	28.016	1.00	41.12	B
ATOM	388	N	DLY	D	1	12.631	-0.899	29.487	1.00	39.74	B
ATOM	389	CA	DLY	D	1	13.997	-0.423	29.356	1.00	37.31	B
ATOM	390	C	DLY	D	1	15.200	-1.051	30.044	1.00	35.38	B
ATOM	391	O	DLY	D	1	15.133	-2.044	30.785	1.00	35.49	B
ATOM	392	N	DLA	D	2	16.332	-0.424	29.752	1.00	33.19	B
ATOM	393	CA	DLA	D	2	17.639	-0.797	30.279	1.00	31.99	B
ATOM	394	CB	DLA	D	2	18.688	0.196	29.762	1.00	31.34	B
ATOM	395	C	DLA	D	2	18.026	-2.217	29.971	1.00	31.71	B
ATOM	396	O	DLA	D	2	18.611	-2.982	30.647	1.00	31.67	B
ATOM	397	N	DCS	D	3	17.699	-2.577	28.640	1.00	30.76	B
ATOM	398	CA	DCS	D	3	18.061	-3.892	28.159	1.00	31.11	B
ATOM	399	C	DCS	D	3	17.104	-4.987	28.618	1.00	31.69	B
ATOM	400	O	DCS	D	3	17.531	-6.020	29.111	1.00	31.85	B
ATOM	401	CB	DCS	D	3	18.128	-3.876	26.638	1.00	30.00	B

Figure 7I

ATOM	402	SG	DCS	D	3	19.502	-2.991	25.840	1.00	30.98	E
ATOM	403	N	DLU	D	4	15.813	-4.736	28.474	1.00	31.68	B
ATOM	404	CA	DLU	D	4	14.782	-5.702	28.834	1.00	32.07	B
ATOM	405	CB	DLU	D	4	13.397	-5.090	28.574	1.00	33.43	B
ATOM	406	CG	DLU	D	4	13.060	-4.844	27.093	1.00	35.53	B
ATOM	407	CD	DLU	D	4	13.663	-3.568	26.500	1.00	36.29	B
ATOM	408	OE1	DLU	D	4	14.422	-2.859	27.182	1.00	37.11	B
ATOM	409	OE2	DLU	D	4	13.367	-3.264	25.323	1.00	37.45	B
ATOM	410	C	DLU	D	4	14.875	-6.180	30.276	1.00	31.86	B
ATOM	411	O	DLU	D	4	14.832	-7.381	30.553	1.00	32.10	B
ATOM	412	N	DLA	D	5	15.022	-5.237	31.196	1.00	30.98	B
ATOM	413	CA	DLA	D	5	15.098	-5.566	32.611	1.00	30.61	B
ATOM	414	CB	DLA	D	5	14.984	-4.296	33.406	1.00	30.83	B
ATOM	415	C	DLA	D	5	16.362	-6.340	33.008	1.00	30.19	B
ATOM	416	O	DLA	D	5	16.387	-7.044	34.027	1.00	30.60	B
ATOM	417	N	DRG	D	6	17.418	-6.202	32.216	1.00	29.09	B
ATOM	418	CA	DRG	D	6	18.673	-6.893	32.489	1.00	28.71	B
ATOM	419	CB	DRG	D	6	18.480	-8.408	32.369	1.00	31.46	B
ATOM	420	CG	DRG	D	6	18.169	-8.847	30.969	1.00	34.88	B
ATOM	421	CD	DRG	D	6	19.397	-8.762	30.070	1.00	37.42	B
ATOM	422	NE	DRG	D	6	19.715	-7.408	29.607	1.00	40.28	B
ATOM	423	CZ	DRG	D	6	20.121	-7.134	28.370	1.00	40.89	B
ATOM	424	NH1	DRG	D	6	20.248	-8.118	27.481	1.00	42.76	B
ATOM	425	NH2	DRG	D	6	20.409	-5.891	28.015	1.00	42.55	B
ATOM	426	C	DRG	D	6	19.313	-6.582	33.833	1.00	27.29	B
ATOM	427	O	DRG	D	6	19.994	-7.423	34.421	1.00	27.43	B
ATOM	428	N	DIS	D	7	19.100	-5.379	34.342	1.00	24.49	B
ATOM	429	CA	DIS	D	7	19.731	-5.018	35.624	1.00	22.04	B
ATOM	430	CB	DIS	D	7	18.970	-3.888	36.284	1.00	22.68	B
ATOM	431	CG	DIS	D	7	17.655	-4.321	36.854	1.00	22.88	B
ATOM	432	CD2	DIS	D	7	17.178	-5.567	37.104	1.00	24.08	B
ATOM	433	ND1	DIS	D	7	16.650	-3.445	37.187	1.00	25.78	B
ATOM	434	CE1	DIS	D	7	15.595	-4.134	37.608	1.00	26.45	B
ATOM	435	NE2	DIS	D	7	15.894	-5.419	37.562	1.00	25.11	B
ATOM	436	C	DIS	D	7	21.156	-4.636	35.329	1.00	21.84	B
ATOM	437	O	DIS	D	7	21.412	-3.743	34.536	1.00	20.32	B
ATOM	438	N	DRG	D	8	22.091	-5.298	36.003	1.00	20.33	B
ATOM	439	CA	DRG	D	8	23.494	-5.122	35.778	1.00	19.80	B
ATOM	440	CB	DRG	D	8	24.284	-5.994	36.755	1.00	20.87	B
ATOM	441	CG	DRG	D	8	24.175	-7.428	36.459	1.00	26.97	B
ATOM	442	CD	DRG	D	8	24.743	-8.207	37.631	1.00	29.07	B
ATOM	443	NE	DRG	D	8	24.581	-9.603	37.325	1.00	31.54	B
ATOM	444	CZ	DRG	D	8	25.258	-10.189	36.352	1.00	31.94	B
ATOM	445	NH1	DRG	D	8	26.139	-9.485	35.658	1.00	33.88	B
ATOM	446	NH2	DRG	D	8	24.987	-11.432	36.027	1.00	33.88	B
ATOM	447	C	DRG	D	8	23.985	-3.711	35.873	1.00	17.95	B
ATOM	448	O	DRG	D	8	24.856	-3.361	35.124	1.00	17.42	B
ATOM	449	N	DLU	D	9	23.407	-2.934	36.783	1.00	16.93	B
ATOM	450	CA	DLU	D	9	23.900	-1.578	36.951	1.00	15.49	B
ATOM	451	CB	DLU	D	9	23.358	-0.954	38.261	1.00	16.03	B
ATOM	452	CG	DLU	D	9	21.876	-0.652	38.323	1.00	16.75	B
ATOM	453	CD	DLU	D	9	20.996	-1.816	38.786	1.00	16.82	B
ATOM	454	OE1	DLU	D	9	21.407	-2.982	38.584	1.00	19.63	B
ATOM	455	OE2	DLU	D	9	19.933	-1.498	39.310	1.00	20.12	B
ATOM	456	C	DLU	D	9	23.601	-0.717	35.747	1.00	15.97	B
ATOM	457	O	DLU	D	9	24.142	0.383	35.655	1.00	15.24	B
ATOM	458	N	DRP	D	10	22.747	-1.186	34.844	1.00	15.66	B
ATOM	459	CA	DRP	D	10	22.462	-0.435	33.611	1.00	15.31	B

Figure 7J

ATOM	460	CB	DRP	D	10	20.960	-0.187	33.420	1.00	16.05	B
ATOM	461	CG	DRP	D	10	20.354	0.791	34.410	1.00	15.28	B
ATOM	462	CD2	DRP	D	10	20.504	2.200	34.384	1.00	15.28	B
ATOM	463	CE2	DRP	D	10	19.734	2.730	35.424	1.00	15.74	B
ATOM	464	CE3	DRP	D	10	21.237	3.075	33.563	1.00	15.47	B
ATOM	465	CD1	DRP	D	10	19.504	0.512	35.449	1.00	16.40	B
ATOM	466	NE1	DRP	D	10	19.122	1.676	36.073	1.00	17.22	B
ATOM	467	CZ2	DRP	D	10	19.650	4.107	35.666	1.00	15.81	B
ATOM	468	CZ3	DRP	D	10	21.174	4.444	33.805	1.00	14.93	B
ATOM	469	CH2	DRP	D	10	20.382	4.935	34.850	1.00	15.26	B
ATOM	470	C	DRP	D	10	23.000	-1.140	32.376	1.00	17.32	B
ATOM	471	O	DRP	D	10	22.790	-0.682	31.244	1.00	16.59	B
ATOM	472	N	DLA	D	11	23.744	-2.227	32.572	1.00	17.72	B
ATOM	473	CA	DLA	D	11	24.253	-2.940	31.407	1.00	18.88	B
ATOM	474	CB	DLA	D	11	25.034	-4.168	31.867	1.00	20.11	B
ATOM	475	C	DLA	D	11	25.126	-2.074	30.501	1.00	18.95	B
ATOM	476	O	DLA	D	11	25.078	-2.221	29.267	1.00	21.13	B
ATOM	477	N	DRP	D	12	25.884	-1.142	31.084	1.00	17.86	B
ATOM	478	CA	DRP	D	12	26.759	-0.275	30.317	1.00	17.72	B
ATOM	479	CB	DRP	D	12	27.586	0.645	31.239	1.00	18.43	B
ATOM	480	CG	DRP	D	12	26.725	1.588	32.059	1.00	16.68	B
ATOM	481	CD2	DRP	D	12	26.285	2.900	31.676	1.00	16.49	B
ATOM	482	CE2	DRP	D	12	25.459	3.371	32.706	1.00	15.68	B
ATOM	483	CE3	DRP	D	12	26.519	3.714	30.561	1.00	17.14	B
ATOM	484	CD1	DRP	D	12	26.177	1.335	33.256	1.00	15.60	B
ATOM	485	NE1	DRP	D	12	25.402	2.400	33.668	1.00	15.74	B
ATOM	486	CZ2	DRP	D	12	24.842	4.628	32.664	1.00	15.78	B
ATOM	487	CZ3	DRP	D	12	25.904	4.977	30.525	1.00	17.42	B
ATOM	488	CH2	DRP	D	12	25.090	5.406	31.550	1.00	16.81	B
ATOM	489	C	DRP	D	12	25.913	0.577	29.346	1.00	18.81	B
ATOM	490	O	DRP	D	12	26.347	0.870	28.231	1.00	20.05	B
ATOM	491	N	DEU	D	13	24.740	1.020	29.790	1.00	17.43	B
ATOM	492	CA	DEU	D	13	23.915	1.866	28.926	1.00	17.59	B
ATOM	493	CB	DEU	D	13	22.883	2.647	29.756	1.00	15.97	B
ATOM	494	CG	DEU	D	13	21.857	3.489	28.971	1.00	15.31	B
ATOM	495	CD1	DEU	D	13	22.559	4.585	28.204	1.00	16.99	B
ATOM	496	CD2	DEU	D	13	20.886	4.105	29.938	1.00	16.07	B
ATOM	497	C	DEU	D	13	23.265	1.011	27.847	1.00	19.32	B
ATOM	498	O	DEU	D	13	23.224	1.429	26.702	1.00	20.12	B
ATOM	499	N	DCS	D	14	22.775	-0.180	28.199	1.00	20.93	B
ATOM	500	CA	DCS	D	14	22.190	-1.046	27.196	1.00	22.79	B
ATOM	501	C	DCS	D	14	23.272	-1.329	26.124	1.00	22.54	B
ATOM	502	O	DCS	D	14	22.963	-1.318	24.916	1.00	23.67	B
ATOM	503	CB	DCS	D	14	21.675	-2.319	27.874	1.00	23.47	B
ATOM	504	SG	DCS	D	14	21.216	-3.669	26.732	1.00	27.91	B
ATOM	505	N	DLA	D	15	24.514	-1.568	26.533	1.00	22.47	B
ATOM	506	CA	DLA	D	15	25.627	-1.857	25.614	1.00	23.31	B
ATOM	507	CB	DLA	D	15	26.868	-2.302	26.401	1.00	24.09	B
ATOM	508	C	DLA	D	15	25.987	-0.672	24.717	1.00	24.16	B
ATOM	509	O	DLA	D	15	26.511	-0.844	23.614	1.00	25.93	B
ATOM	510	N	DLA	D	16	25.723	0.544	25.192	1.00	22.60	B
ATOM	511	CA	DLA	D	16	26.017	1.743	24.400	1.00	22.10	B
ATOM	512	CB	DLA	D	16	26.006	2.985	25.314	1.00	22.02	B
ATOM	513	C	DLA	D	16	24.995	1.932	23.278	1.00	21.95	B
ATOM	514	O	DLA	D	16	25.355	2.570	22.256	1.00	22.36	B
ATOM	515	NT	DLA	D	16	23.843	1.460	23.410	1.00	23.47	B
ATOM	516	CL-1	CL	I	1	20.914	12.075	1.899	1.00	45.04	I
ATOM	517	OH2	WAT	W	1	23.911	6.454	-21.684	1.00	53.50	W

Figure 7K

ATOM	518	OH2 WAT W	2	30.822	2.444	-19.357	1.00	52.17	W
ATOM	519	OH2 WAT W	3	30.369	13.971	-17.693	1.00	37.33	W
ATOM	520	OH2 WAT W	4	27.699	12.875	-16.588	1.00	46.63	W
ATOM	521	OH2 WAT W	5	23.417	1.727	-13.168	1.00	48.41	W
ATOM	522	OH2 WAT W	6	24.012	1.401	-16.007	1.00	58.65	W
ATOM	523	OH2 WAT W	7	16.572	3.069	-7.418	1.00	36.12	W
ATOM	524	OH2 WAT W	8	32.381	11.028	-8.334	1.00	55.01	W
ATOM	525	OH2 WAT W	9	33.753	7.275	-10.261	1.00	53.14	W
ATOM	526	OH2 WAT W	10	20.318	-0.862	-12.067	1.00	28.89	W
ATOM	527	OH2 WAT W	11	26.434	1.459	-10.129	1.00	43.04	W
ATOM	528	OH2 WAT W	12	27.878	0.323	-12.146	1.00	55.95	W
ATOM	529	OH2 WAT W	13	31.427	0.259	-10.741	1.00	52.47	W
ATOM	530	OH2 WAT W	14	29.889	8.411	-6.889	1.00	56.49	W
ATOM	531	OH2 WAT W	15	22.532	1.843	-4.021	1.00	32.19	W
ATOM	532	OH2 WAT W	16	23.814	-0.534	-4.336	1.00	39.56	W
ATOM	533	OH2 WAT W	17	19.996	1.598	-5.292	1.00	33.28	W
ATOM	534	OH2 WAT W	18	25.262	-3.040	-8.386	1.00	28.37	W
ATOM	535	OH2 WAT W	19	22.556	0.000	0.001	1.00	30.95	W
ATOM	536	OH2 WAT W	20	24.369	-1.421	-1.823	1.00	29.32	W
ATOM	537	OH2 WAT W	21	29.134	-0.583	-6.291	1.00	46.18	W
ATOM	538	OH2 WAT W	22	27.394	2.286	-5.533	1.00	43.67	W
ATOM	539	OH2 WAT W	23	26.774	0.049	-4.387	1.00	45.47	W
ATOM	540	OH2 WAT W	24	30.008	5.236	1.507	1.00	52.80	W
ATOM	541	OH2 WAT W	25	27.776	4.560	0.356	1.00	42.94	W
ATOM	542	OH2 WAT W	26	32.018	6.237	0.261	1.00	53.15	W
ATOM	543	OH2 WAT W	28	18.650	4.426	-0.423	1.00	34.71	W
ATOM	544	OH2 WAT W	29	18.919	1.842	-1.284	1.00	42.23	W
ATOM	545	OH2 WAT W	30	11.826	6.239	7.700	1.00	59.49	W
ATOM	546	OH2 WAT W	31	13.683	5.469	2.919	1.00	52.76	W
ATOM	547	OH2 WAT W	32	16.956	4.594	1.380	1.00	47.84	W
ATOM	548	OH2 WAT W	33	17.260	2.099	7.679	1.00	46.32	W
ATOM	549	OH2 WAT W	34	17.636	1.737	-4.073	1.00	51.94	W
ATOM	550	OH2 WAT W	35	16.221	5.835	9.764	1.00	30.19	W
ATOM	551	OH2 WAT W	36	26.030	8.926	8.979	1.00	51.32	W
ATOM	552	OH2 WAT W	37	13.758	2.898	9.624	1.00	52.05	W
ATOM	553	OH2 WAT W	38	14.899	5.914	11.925	1.00	35.86	W
ATOM	554	OH2 WAT W	39	19.841	0.030	14.724	1.00	45.90	W
ATOM	555	OH2 WAT W	40	13.772	2.335	12.179	1.00	50.60	W
ATOM	556	OH2 WAT W	41	13.367	0.805	6.229	1.00	51.80	W
ATOM	557	OH2 WAT W	42	15.587	3.501	15.845	1.00	30.05	W
ATOM	558	OH2 WAT W	43	14.280	4.098	13.819	1.00	48.74	W
ATOM	559	OH2 WAT W	44	14.273	3.983	18.042	1.00	32.62	W
ATOM	560	OH2 WAT W	45	14.275	2.720	20.720	1.00	40.19	W
ATOM	561	OH2 WAT W	46	21.969	2.228	18.885	1.00	22.32	W
ATOM	562	OH2 WAT W	47	21.588	1.778	21.594	1.00	28.43	W
ATOM	563	OH2 WAT W	48	11.908	3.300	22.023	1.00	50.50	W
ATOM	564	OH2 WAT W	49	13.679	0.626	18.643	1.00	46.64	W
ATOM	565	OH2 WAT W	50	16.369	2.196	22.597	1.00	30.08	W
ATOM	566	OH2 WAT W	51	12.828	6.527	18.634	1.00	37.29	W
ATOM	567	OH2 WAT W	52	24.603	2.631	19.581	1.00	25.55	W
ATOM	568	OH2 WAT W	53	11.867	0.791	23.131	1.00	58.27	W
ATOM	569	OH2 WAT W	54	24.646	5.366	17.812	1.00	50.24	W
ATOM	570	OH2 WAT W	55	20.954	0.091	17.131	1.00	49.14	W
ATOM	571	OH2 WAT W	56	19.747	-0.562	21.394	1.00	36.92	W
ATOM	572	OH2 WAT W	57	14.819	8.442	19.922	1.00	33.61	W
ATOM	573	OH2 WAT W	58	10.854	5.349	19.724	1.00	45.89	W
ATOM	574	OH2 WAT W	59	10.710	9.378	19.376	1.00	37.52	W
ATOM	575	OH2 WAT W	60	10.497	10.303	21.845	1.00	34.96	W

Figure 7L

ATOM	576	OH2 WAT W	61	12.866	5.691	26.354	1.00	28.86	W
ATOM	577	OH2 WAT W	62	10.758	7.878	25.495	1.00	42.32	W
ATOM	578	OH2 WAT W	63	11.782	6.555	28.773	1.00	29.65	W
ATOM	579	OH2 WAT W	64	10.296	8.472	27.988	1.00	37.31	W
ATOM	580	OH2 WAT W	65	13.316	2.342	26.849	1.00	43.22	W
ATOM	581	OH2 WAT W	66	29.863	-1.693	28.654	1.00	38.41	W
ATOM	582	OH2 WAT W	67	16.468	-1.186	26.444	1.00	32.71	W
ATOM	583	OH2 WAT W	68	20.934	12.065	25.212	1.00	18.68	W
ATOM	584	OH2 WAT W	69	7.101	5.989	26.485	1.00	48.02	W
ATOM	585	OH2 WAT W	70	7.226	10.744	27.574	1.00	33.30	W
ATOM	586	OH2 WAT W	71	16.382	-1.374	34.997	1.00	34.36	W
ATOM	587	OH2 WAT W	72	17.474	-0.717	38.167	1.00	28.82	W
ATOM	588	OH2 WAT W	73	17.984	-2.951	33.186	1.00	27.39	W
ATOM	589	OH2 WAT W	74	16.999	1.929	37.830	1.00	37.09	W
ATOM	590	OH2 WAT W	75	20.595	3.071	39.121	1.00	19.51	W
ATOM	591	OH2 WAT W	76	14.326	5.004	39.584	1.00	20.31	W
ATOM	592	OH2 WAT W	77	11.973	4.544	38.034	1.00	32.93	W
ATOM	593	OH2 WAT W	78	18.317	4.417	39.397	1.00	44.00	W
ATOM	594	OH2 WAT W	79	10.983	-2.804	30.948	1.00	52.39	W
ATOM	595	OH2 WAT W	80	11.064	0.945	32.640	1.00	30.78	W
ATOM	596	OH2 WAT W	81	12.861	0.902	39.566	1.00	51.74	W
ATOM	597	OH2 WAT W	82	14.353	-1.379	39.210	1.00	48.06	W
ATOM	598	OH2 WAT W	83	13.014	-3.417	36.263	1.00	46.54	W
ATOM	599	OH2 WAT W	84	11.101	-2.319	39.669	1.00	61.24	W
ATOM	600	OH2 WAT W	85	20.879	-3.825	31.838	1.00	26.25	W
ATOM	601	OH2 WAT W	86	24.470	-4.753	28.192	1.00	36.86	W
ATOM	602	OH2 WAT W	87	22.117	-5.700	29.831	1.00	38.03	W
ATOM	603	OH2 WAT W	88	19.685	0.721	41.041	1.00	28.21	W
ATOM	604	OH2 WAT W	89	20.274	5.127	40.337	1.00	32.29	W
ATOM	605	OH2 WAT W	90	10.072	4.538	29.943	1.00	33.10	W
ATOM	606	OH2 WAT W	91	10.573	4.216	33.496	1.00	33.22	W
ATOM	607	OH2 WAT W	92	10.336	5.922	36.364	1.00	48.48	W
ATOM	608	OH2 WAT W	93	9.113	5.209	40.332	1.00	51.71	W
ATOM	609	OH2 WAT W	94	9.980	8.713	42.573	1.00	24.98	W
ATOM	610	OH2 WAT W	95	17.708	6.542	-1.798	1.00	36.93	W
ATOM	611	OH2 WAT W	96	10.278	11.397	38.730	1.00	17.13	W
ATOM	612	OH2 WAT W	97	11.290	10.478	36.184	1.00	15.62	W
ATOM	613	OH2 WAT W	98	8.444	12.988	37.395	1.00	17.25	W
ATOM	614	OH2 WAT W	99	8.735	9.911	40.361	1.00	25.18	W
ATOM	615	OH2 WAT W	100	6.665	11.917	35.865	1.00	28.95	W
ATOM	616	OH2 WAT W	101	8.907	9.736	35.113	1.00	28.77	W
ATOM	617	OH2 WAT W	102	10.416	5.919	42.300	1.00	32.80	W
ATOM	618	OH2 WAT W	103	8.278	3.600	38.536	1.00	54.85	W
ATOM	619	OH2 WAT W	104	14.183	7.249	45.734	1.00	23.53	W
ATOM	620	OH2 WAT W	105	11.426	7.965	46.547	1.00	34.68	W
ATOM	621	OH2 WAT W	106	16.907	2.218	41.970	1.00	39.50	W
ATOM	622	OH2 WAT W	107	16.479	14.336	46.761	1.00	23.72	W
ATOM	623	OH2 WAT W	108	8.319	12.931	45.022	1.00	22.11	W
ATOM	624	OH2 WAT W	109	7.189	12.423	42.385	1.00	39.34	W
ATOM	625	OH2 WAT W	110	8.599	9.769	44.603	1.00	40.15	W
ATOM	626	OH2 WAT W	111	26.891	-1.858	33.829	1.00	23.69	W
ATOM	627	OH2 WAT W	112	28.775	-3.310	32.521	1.00	38.13	W
ATOM	628	OH2 WAT W	113	31.335	0.587	33.068	1.00	34.37	W
ATOM	629	OH2 WAT W	114	30.921	-0.919	36.513	1.00	44.24	W
ATOM	630	OH2 WAT W	115	30.098	2.733	29.619	1.00	39.50	W
ATOM	631	OH2 WAT W	116	33.465	2.665	34.521	1.00	52.27	W
ATOM	632	OH2 WAT W	117	25.612	14.159	-18.301	1.00	56.10	W
ATOM	633	OH2 WAT W	118	33.904	2.165	-15.960	1.00	57.70	W

Figure 7M

ATOM	634	OH2	WAT	W	119	33.766	4.315	-14.106	1.00	57.44	W
ATOM	635	OH2	WAT	W	120	26.831	7.497	7.075	1.00	40.38	W
ATOM	636	OH2	WAT	W	121	26.562	8.206	4.240	1.00	32.00	W
ATOM	637	OH2	WAT	W	122	29.081	7.039	3.251	1.00	46.30	W
ATOM	638	OH2	WAT	W	123	22.080	-0.975	10.516	1.00	39.31	W
ATOM	639	OH2	WAT	W	124	28.185	3.991	13.044	1.00	45.28	W
ATOM	640	OH2	WAT	W	125	29.400	7.324	10.996	1.00	52.21	W
ATOM	641	OH2	WAT	W	126	12.966	3.595	24.673	1.00	59.42	W
ATOM	642	OH2	WAT	W	127	8.932	7.961	36.476	1.00	45.85	W
ATOM	643	OH2	WAT	W	128	12.712	5.206	41.719	1.00	38.55	W
ATOM	644	OH2	WAT	W	129	9.431	10.564	47.230	1.00	35.27	W
ATOM	645	OH2	WAT	W	130	6.643	9.576	45.596	1.00	44.00	W
ATOM	646	OH2	WAT	W	131	21.501	13.657	45.856	1.00	43.49	W
ATOM	647	OH2	WAT	W	132	19.368	14.112	46.567	1.00	41.15	W
ATOM	648	OH2	WAT	W	133	20.913	12.058	48.230	1.00	36.86	W
ATOM	649	OH2	WAT	W	134	13.556	4.967	44.137	1.00	49.55	W
ATOM	650	OH2	WAT	W	135	17.568	0.000	0.010	1.00	54.94	W
ATOM	651	OH2	WAT	W	136	17.847	-0.139	11.093	1.00	42.03	W
ATOM	652	OH2	WAT	W	137	25.734	4.074	15.641	1.00	35.36	W
ATOM	653	OH2	WAT	W	138	8.107	7.930	38.831	1.00	37.47	W
ATOM	654	OH2	WAT	W	139	10.614	4.603	44.378	1.00	61.10	W
ATOM	655	OH2	WAT	W	140	14.180	-9.552	32.610	1.00	37.66	W
ATOM	656	OH2	WAT	W	141	26.549	-4.072	22.858	1.00	48.05	W
ATOM	657	OH2	WAT	W	142	21.688	-2.141	22.847	1.00	36.75	W
ATOM	658	OH2	WAT	W	143	15.457	1.462	27.799	1.00	38.11	W
ATOM	659	OH2	WAT	W	144	18.956	16.356	45.521	1.00	36.93	W
ATOM	660	OH2	WAT	W	145	15.655	2.938	40.183	1.00	40.77	W
ATOM	661	OH2	WAT	W	146	15.688	-1.613	19.777	1.00	47.04	W
ATOM	662	OH2	WAT	W	147	26.880	-5.627	28.327	1.00	44.89	W
ATOM	663	OH2	WAT	W	148	28.682	-5.605	33.707	1.00	43.34	W
ATOM	664	OH2	WAT	W	149	28.220	11.179	-23.836	1.00	53.67	W
ATOM	665	OH2	WAT	W	150	27.905	3.222	-7.774	1.00	44.54	W
ATOM	666	OH2	WAT	W	151	15.403	-11.541	32.995	1.00	47.59	W
TER											
END											

Figure 7N

Inhibition of HIV-1 Membrane Fusion by a D-Peptide

Figure 8A
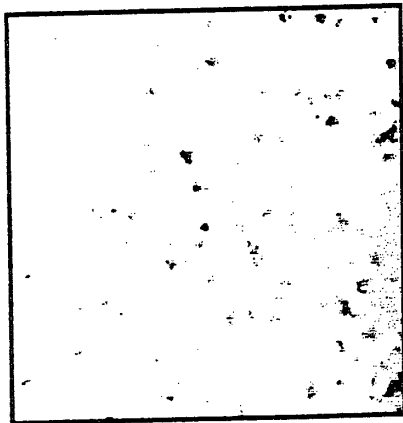
Figure 8B

Syncytia Assay with no D-peptide
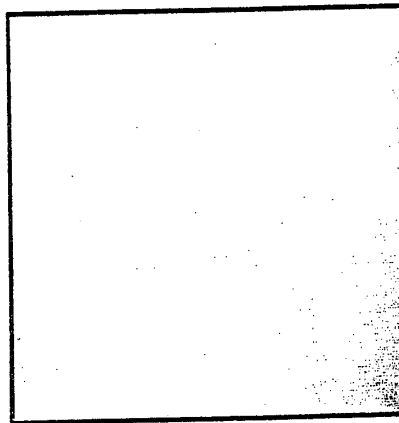
Syncytia Assay with [100 μM] peptide

NMR Charact rization of Aromatic Residues in
IQN17/D-Peptide Complexes
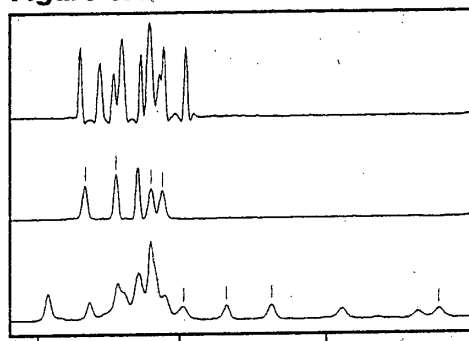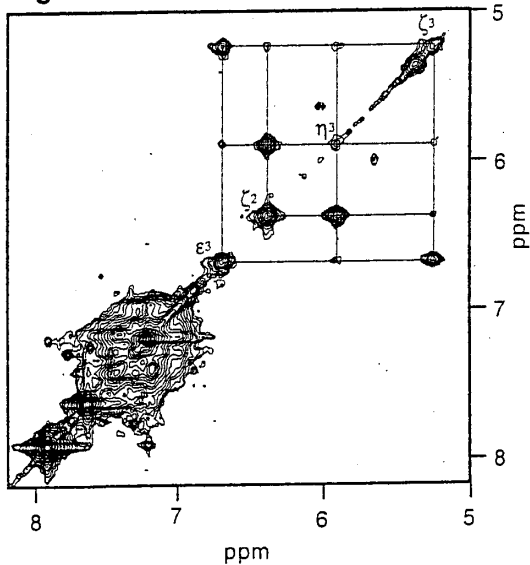
Figure 9A
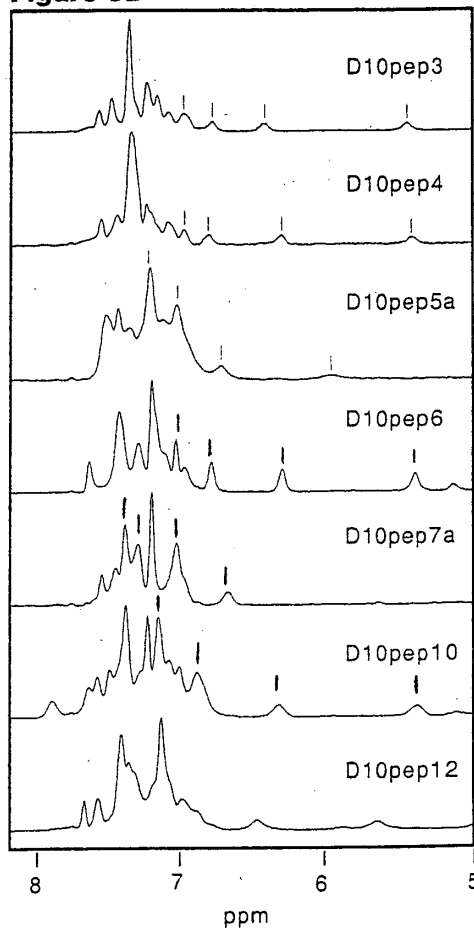
Figure 9B

Figure 9C

Figure 10: Conformation of D10pep1 in complex with IQN17
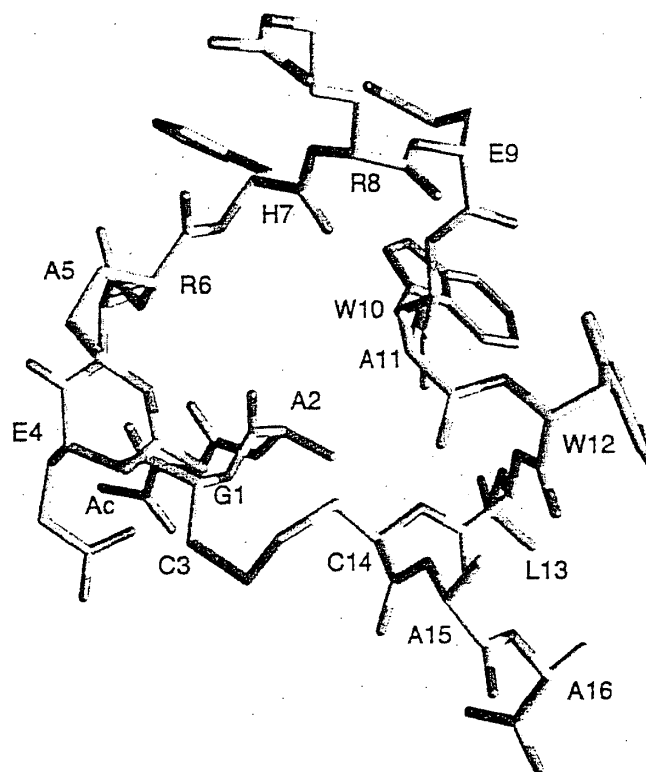
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CRYST1    57.935  121.959   73.669  90.00   90.00   90.00 C2221          1
ORIGX1       1.000000  0.000000  0.000000        0.00000
ORIGX2       0.000000  1.000000  0.000000        0.00000
ORIGX3       0.000000  0.000000  1.000000        0.00000
SCALE1       0.017261  0.000000  0.000000        0.00000
SCALE2       0.000000  0.008199  0.000000        0.00000
SCALE3       0.000000  0.000000  0.013574        0.00000
ATOM      1  CA  ACE A   0      25.795  17.140  37.286  1.00 61.88      A
ATOM      2  C   ACE A   0      25.799  18.376  36.435  1.00 62.00      A
ATOM      3  O   ACE A   0      25.500  19.475  36.921  1.00 62.10      A
ATOM      4  N   ARG A   1      26.134  18.217  35.157  1.00 60.34      A
ATOM      5  CA  ARG A   1      26.203  19.328  34.217  1.00 60.56      A
ATOM      6  CB  ARG A   1      27.212  18.993  33.110  1.00 61.87      A
ATOM      7  CG  ARG A   1      27.630  20.135  32.212  1.00 60.78      A
ATOM      8  CD  ARG A   1      28.500  19.587  31.097  1.00 64.25      A
ATOM      9  NE  ARG A   1      29.018  20.628  30.217  1.00 65.07      A
ATOM     10  CZ  ARG A   1      29.706  20.377  29.109  1.00 63.90      A
ATOM     11  NH1 ARG A   1      29.951  19.124  28.766  1.00 64.20      A
ATOM     12  NH2 ARG A   1      30.157  21.367  28.351  1.00 63.51      A
ATOM     13  C   ARG A   1      24.823  19.573  33.595  1.00 59.45      A
ATOM     14  O   ARG A   1      24.453  20.714  33.294  1.00 57.69      A
ATOM     15  N   MET A   2      24.065  18.494  33.425  1.00 57.60      A
ATOM     16  CA  MET A   2      22.736  18.573  32.836  1.00 59.85      A
ATOM     17  CB  MET A   2      22.273  17.198  32.397  1.00 59.85      A
ATOM     18  CG  MET A   2      21.204  17.251  31.342  1.00 63.56      A
ATOM     19  SD  MET A   2      20.044  15.905  31.454  1.00 67.77      A
ATOM     20  CE  MET A   2      19.089  16.438  32.857  1.00 66.61      A
ATOM     21  C   MET A   2      21.723  19.130  33.834  1.00 61.33      A
ATOM     22  O   MET A   2      20.543  19.276  33.521  1.00 59.97      A
ATOM     23  N   LYS A   3      22.200  19.417  35.041  1.00 62.71      A
ATOM     24  CA  LYS A   3      21.373  19.961  36.107  1.00 63.07      A
ATOM     25  CB  LYS A   3      21.817  19.361  37.449  1.00 64.25      A
ATOM     26  CG  LYS A   3      20.982  19.721  38.687  1.00 64.89      A
ATOM     27  CD  LYS A   3      21.195  21.159  39.160  1.00 64.67      A
ATOM     28  CE  LYS A   3      20.543  21.405  40.525  1.00 64.66      A
ATOM     29  NZ  LYS A   3      19.077  21.123  40.548  1.00 63.04      A
ATOM     30  C   LYS A   3      21.599  21.467  36.062  1.00 64.55      A
ATOM     31  O   LYS A   3      20.639  22.245  36.032  1.00 64.65      A
ATOM     32  N   GLN A   4      22.869  21.873  36.036  1.00 64.34      A
ATOM     33  CA  GLN A   4      23.232  23.289  35.952  1.00 65.46      A
ATOM     34  CB  GLN A   4      24.746  23.447  35.780  1.00 67.71      A
ATOM     35  CG  GLN A   4      25.552  22.954  36.963  1.00 71.16      A
ATOM     36  CD  GLN A   4      25.297  23.771  38.212  1.00 75.18      A
ATOM     37  OE1 GLN A   4      25.618  24.962  38.269  1.00 77.70      A
ATOM     38  NE2 GLN A   4      24.706  23.135  39.225  1.00 76.77      A
ATOM     39  C   GLN A   4      22.508  23.928  34.758  1.00 64.11      A
ATOM     40  O   GLN A   4      22.191  25.128  34.776  1.00 62.08      A
ATOM     41  N   ILE A   5      22.260  23.120  33.726  1.00 59.80      A
ATOM     42  CA  ILE A   5      21.540  23.587  32.552  1.00 58.22      A
ATOM     43  CB  ILE A   5      21.567  22.558  31.398  1.00 56.35      A
ATOM     44  CG2 ILE A   5      20.438  22.851  30.416  1.00 53.92      A
ATOM     45  CG1 ILE A   5      22.942  22.562  30.719  1.00 56.47      A
ATOM     46  CD1 ILE A   5      23.079  21.524  29.614  1.00 59.50      A
ATOM     47  C   ILE A   5      20.083  23.828  32.929  1.00 58.98      A
ATOM     48  O   ILE A   5      19.575  24.928  32.729  1.00 58.48      A
ATOM     49  N   GLU A   6      19.424  22.796  33.472  1.00 59.29      A
ATOM     50  CA  GLU A   6      18.013  22.883  33.377  1.00 56.51      A
ATOM     51  CB  GLU A   6      17.529  21.637  34.449  1.00 55.59      A
```

Figure 11A

ATOM	52	CG	GLU	A	6	17.638	20.359	33.480	1.00	56.46	A
ATOM	53	CD	GLU	A	6	17.293	19.009	34.119	1.00	56.33	A
ATOM	54	OE1	GLU	A	6	17.702	18.790	35.278	1.00	53.43	A
ATOM	55	OE2	GLU	A	6	16.644	18.157	33.458	1.00	55.03	A
ATOM	56	C	GLU	A	6	17.873	23.977	34.926	1.00	54.87	A
ATOM	57	O	GLU	A	6	16.793	24.509	35.137	1.00	52.82	A
ATOM	58	N	ASP	A	7	18.986	24.300	35.572	1.00	55.62	A
ATOM	59	CA	ASP	A	7	19.039	25.336	36.597	1.00	56.65	A
ATOM	60	CB	ASP	A	7	20.291	25.162	37.451	1.00	57.46	A
ATOM	61	CG	ASP	A	7	20.010	24.471	38.762	1.00	57.37	A
ATOM	62	OD1	ASP	A	7	19.180	23.534	38.775	1.00	53.78	A
ATOM	63	OD2	ASP	A	7	20.637	24.862	39.771	1.00	57.66	A
ATOM	64	C	ASP	A	7	19.034	26.745	36.041	1.00	56.99	A
ATOM	65	O	ASP	A	7	18.516	27.662	36.678	1.00	55.43	A
ATOM	66	N	LYS	A	8	19.632	26.945	34.873	1.00	58.30	A
ATOM	67	CA	LYS	A	8	19.642	28.290	34.312	1.00	59.87	A
ATOM	68	CB	LYS	A	8	20.971	28.599	33.612	1.00	62.61	A
ATOM	69	CG	LYS	A	8	22.203	28.372	34.487	1.00	66.85	A
ATOM	70	CD	LYS	A	8	23.232	29.498	34.357	1.00	70.21	A
ATOM	71	CE	LYS	A	8	22.915	30.676	35.293	1.00	72.00	A
ATOM	72	NZ	LYS	A	8	21.583	31.323	35.091	1.00	72.05	A
ATOM	73	C	LYS	A	8	18.467	28.481	33.354	1.00	58.08	A
ATOM	74	O	LYS	A	8	18.145	29.609	32.969	1.00	56.44	A
ATOM	75	N	ILE	A	9	17.835	27.376	32.967	1.00	55.29	A
ATOM	76	CA	ILE	A	9	16.668	27.436	32.099	1.00	56.69	A
ATOM	77	CB	ILE	A	9	16.325	26.052	31.486	1.00	54.89	A
ATOM	78	CG2	ILE	A	9	14.892	26.067	30.915	1.00	54.20	A
ATOM	79	CG1	ILE	A	9	17.373	25.676	30.423	1.00	55.96	A
ATOM	80	CD1	ILE	A	9	17.131	24.339	29.717	1.00	54.22	A
ATOM	81	C	ILE	A	9	15.526	27.876	33.018	1.00	57.98	A
ATOM	82	O	ILE	A	9	14.603	28.572	32.616	1.00	55.85	A
ATOM	83	N	GLU	A	10	15.626	27.458	34.271	1.00	59.96	A
ATOM	84	CA	GLU	A	10	14.641	27.788	35.283	1.00	61.12	A
ATOM	85	CB	GLU	A	10	14.850	26.901	36.510	1.00	63.01	A
ATOM	86	CG	GLU	A	10	13.846	27.117	37.618	1.00	66.89	A
ATOM	87	CD	GLU	A	10	14.387	26.672	38.955	1.00	68.37	A
ATOM	88	OE1	GLU	A	10	14.844	25.510	39.054	1.00	67.70	A
ATOM	89	OE2	GLU	A	10	14.355	27.487	39.903	1.00	68.42	A
ATOM	90	C	GLU	A	10	14.872	29.243	35.664	1.00	59.41	A
ATOM	91	O	GLU	A	10	13.947	29.958	36.037	1.00	59.95	A
ATOM	92	N	GLU	A	11	16.127	29.663	35.565	1.00	57.16	A
ATOM	93	CA	GLU	A	11	16.524	31.024	35.893	1.00	55.88	A
ATOM	94	CB	GLU	A	11	18.042	31.095	36.019	1.00	58.17	A
ATOM	95	CG	GLU	A	11	18.569	32.375	36.627	1.00	62.73	A
ATOM	96	CD	GLU	A	11	18.459	32.382	38.139	1.00	67.75	A
ATOM	97	OE1	GLU	A	11	19.101	31.512	38.782	1.00	67.91	A
ATOM	98	OE2	GLU	A	11	17.736	33.249	38.681	1.00	68.84	A
ATOM	99	C	GLU	A	11	16.056	31.976	34.789	1.00	54.76	A
ATOM	100	O	GLU	A	11	15.805	33.160	35.030	1.00	54.78	A
ATOM	101	N	ILE	A	12	15.945	31.443	33.575	1.00	52.61	A
ATOM	102	CA	ILE	A	12	15.510	32.210	32.414	1.00	50.09	A
ATOM	103	CB	ILE	A	12	16.002	31.548	31.096	1.00	50.23	A
ATOM	104	CG2	ILE	A	12	15.201	32.073	29.905	1.00	48.54	A
ATOM	105	CG1	ILE	A	12	17.508	31.773	30.930	1.00	50.30	A
ATOM	106	CD1	ILE	A	12	18.114	31.062	29.724	1.00	53.10	A
ATOM	107	C	ILE	A	12	13.988	32.324	32.362	1.00	49.83	A
ATOM	108	O	ILE	A	12	13.447	33.376	32.017	1.00	47.70	A
ATOM	109	N	GLU	A	13	13.306	31.233	32.698	1.00	48.57	A
ATOM	110	CA	GLU	A	13	11.849	31.218	32.677	1.00	48.22	A
ATOM	111	CB	GLU	A	13	11.320	29.810	32.954	1.00	45.44	A

Figure 11B

ATOM	112	CG	GLU A	13	11.673	28.794	31.895	1.00 46.65	A
ATOM	113	CD	GLU A	13	11.419	27.372	32.358	1.00 49.90	A
ATOM	114	OE1	GLU A	13	12.051	26.968	33.366	1.00 49.96	A
ATOM	115	OE2	GLU A	13	10.599	26.665	31.720	1.00 50.18	A
ATOM	116	C	GLU A	13	11.357	32.163	33.749	1.00 47.83	A
ATOM	117	O	GLU A	13	10.279	32.731	33.638	1.00 48.72	A
ATOM	118	N	SER A	14	12.168	32.313	34.786	1.00 48.67	A
ATOM	119	CA	SER A	14	11.862	33.187	35.907	1.00 49.89	A
ATOM	120	CB	SER A	14	12.906	32.985	37.014	1.00 49.05	A
ATOM	121	OG	SER A	14	12.634	33.773	38.160	1.00 49.35	A
ATOM	122	C	SER A	14	11.885	34.627	35.415	1.00 50.52	A
ATOM	123	O	SER A	14	10.869	35.313	35.431	1.00 54.15	A
ATOM	124	N	LYS A	15	13.056	35.067	34.971	1.00 49.27	A
ATOM	125	CA	LYS A	15	13.248	36.416	34.474	1.00 51.02	A
ATOM	126	CB	LYS A	15	14.707	36.589	34.042	1.00 54.30	A
ATOM	127	CG	LYS A	15	15.018	37.931	33.417	1.00 58.79	A
ATOM	128	CD	LYS A	15	14.843	39.039	34.437	1.00 63.42	A
ATOM	129	CE	LYS A	15	15.841	38.880	35.576	1.00 65.66	A
ATOM	130	NZ	LYS A	15	15.722	39.983	36.569	1.00 68.14	A
ATOM	131	C	LYS A	15	12.313	36.758	33.305	1.00 50.99	A
ATOM	132	O	LYS A	15	12.022	37.926	33.061	1.00 49.62	A
ATOM	133	N	GLN A	16	11.848	35.740	32.587	1.00 50.06	A
ATOM	134	CA	GLN A	16	10.965	35.937	31.444	1.00 49.96	A
ATOM	135	CB	GLN A	16	10.950	34.684	30.570	1.00 49.89	A
ATOM	136	CG	GLN A	16	10.133	34.810	29.286	1.00 50.59	A
ATOM	137	CD	GLN A	16	10.287	33.603	28.369	1.00 54.27	A
ATOM	138	OE1	GLN A	16	9.799	32.511	28.667	1.00 56.28	A
ATOM	139	NE2	GLN A	16	10.985	33.796	27.250	1.00 54.69	A
ATOM	140	C	GLN A	16	9.551	36.256	31.899	1.00 50.61	A
ATOM	141	O	GLN A	16	8.788	36.931	31.195	1.00 48.56	A
ATOM	142	N	LYS A	17	9.198	35.736	33.067	1.00 49.38	A
ATOM	143	CA	LYS A	17	7.883	35.973	33.623	1.00 49.73	A
ATOM	144	CB	LYS A	17	7.582	34.982	34.750	1.00 52.97	A
ATOM	145	CG	LYS A	17	6.250	35.226	35.448	1.00 56.86	A
ATOM	146	CD	LYS A	17	6.066	34.276	36.618	1.00 59.31	A
ATOM	147	CE	LYS A	17	4.763	34.552	37.354	1.00 59.95	A
ATOM	148	NZ	LYS A	17	4.592	33.621	38.506	1.00 62.05	A
ATOM	149	C	LYS A	17	7.927	37.390	34.163	1.00 48.25	A
ATOM	150	O	LYS A	17	6.977	38.144	34.008	1.00 47.73	A
ATOM	151	N	LYS A	18	9.043	37.750	34.791	1.00 45.58	A
ATOM	152	CA	LYS A	18	9.190	39.101	35.309	1.00 45.26	A
ATOM	153	CB	LYS A	18	10.523	39.270	36.047	1.00 47.34	A
ATOM	154	CG	LYS A	18	10.627	38.493	37.362	1.00 50.10	'A
ATOM	155	CD	LYS A	18	11.831	38.976	38.168	1.00 52.93	A
ATOM	156	CE	LYS A	18	11.869	38.358	39.550	1.00 55.07	A
ATOM	157	NZ	LYS A	18	12.933	38.968	40.398	1.00 59.20	A
ATOM	158	C	LYS A	18	9.107	40.110	34.171	1.00 41.59	A
ATOM	159	O	LYS A	18	8.585	41.206	34.349	1.00 42.70	A
ATOM	160	N	ILE A	19	9.633	39.740	33.008	1.00 40.25	A
ATOM	161	CA	ILE A	19	9.605	40.595	31.831	1.00 39.53	A
ATOM	162	CB	ILE A	19	10.494	40.015	30.710	1.00 42.08	A
ATOM	163	CG2	ILE A	19	10.133	40.631	29.369	1.00 41.71	A
ATOM	164	CG1	ILE A	19	11.969	40.214	31.074	1.00 42.52	A
ATOM	165	CD1	ILE A	19	12.939	39.656	30.039	1.00 43.29	A
ATOM	166	C	ILE A	19	8.172	40.725	31.325	1.00 39.27	A
ATOM	167	O	ILE A	19	7.751	41.790	30.899	1.00 37.81	A
ATOM	168	N	GLU A	20	7.421	39.637	31.372	1.00 39.00	A
ATOM	169	CA	GLU A	20	6.036	39.692	30.930	1.00 40.27	A
ATOM	170	CB	GLU A	20	5.437	38.280	30.834	1.00 43.21	A
ATOM	171	CG	GLU A	20	5.898	37.474	29.606	1.00 48.10	A

Figure 11C

ATOM	172	CD	GLU A	20	5.446	36.019	29.659	1.00	50.57	A
ATOM	173	OE1	GLU A	20	5.832	35.316	30.617	1.00	52.42	A
ATOM	174	OE2	GLU A	20	4.708	35.575	28.752	1.00	52.16	A
ATOM	175	C	GLU A	20	5.195	40.546	31.873	1.00	40.09	A
ATOM	176	O	GLU A	20	4.148	41.056	31.480	1.00	40.96	A
ATOM	177	N	ASN A	21	5.637	40.694	33.119	1.00	38.83	A
ATOM	178	CA	ASN A	21	4.880	41.498	34.071	1.00	40.69	A
ATOM	179	CB	ASN A	21	5.216	41.107	35.507	1.00	39.42	A
ATOM	180	CG	ASN A	21	4.618	39.768	35.892	1.00	41.35	A
ATOM	181	OD1	ASN A	21	3.905	39.151	35.102	1.00	38.98	A
ATOM	182	ND2	ASN A	21	4.902	39.312	37.107	1.00	40.82	A
ATOM	183	C	ASN A	21	5.163	42.958	33.846	1.00	42.25	A
ATOM	184	O	ASN A	21	4.261	43.801	33.872	1.00	42.61	A
ATOM	185	N	GLU A	22	6.432	43.244	33.602	1.00	41.94	A
ATOM	186	CA	GLU A	22	6.893	44.589	33.343	1.00	41.44	A
ATOM	187	CB	GLU A	22	8.403	44.563	33.127	1.00	43.01	A
ATOM	188	CG	GLU A	22	9.126	45.861	33.421	1.00	49.75	A
ATOM	189	CD	GLU A	22	9.769	45.872	34.802	1.00	52.80	A
ATOM	190	OE1	GLU A	22	10.611	44.988	35.077	1.00	53.66	A
ATOM	191	OE2	GLU A	22	9.447	46.764	35.608	1.00	57.41	A
ATOM	192	C	GLU A	22	6.188	45.082	32.068	1.00	41.34	A
ATOM	193	O	GLU A	22	5.851	46.263	31.954	1.00	43.52	A
ATOM	194	N	ILE A	23	5.964	44.175	31.116	1.00	37.55	A
ATOM	195	CA	ILE A	23	5.295	44.530	29.863	1.00	35.10	A
ATOM	196	CB	ILE A	23	5.418	43.408	28.800	1.00	36.19	A
ATOM	197	CG2	ILE A	23	4.520	43.719	27.592	1.00	35.94	A
ATOM	198	CG1	ILE A	23	6.876	43.288	28.340	1.00	39.18	A
ATOM	199	CD1	ILE A	23	7.122	42.193	27.324	1.00	40.80	A
ATOM	200	C	ILE A	23	3.816	44.827	30.093	1.00	33.36	A
ATOM	201	O	ILE A	23	3.284	45.796	29.568	1.00	28.55	A
ATOM	202	N	ALA A	24	3.167	43.981	30.881	1.00	30.41	A
ATOM	203	CA	ALA A	24	1.760	44.147	31.179	1.00	30.11	A
ATOM	204	CB	ALA A	24	1.276	42.994	32.043	1.00	27.29	A
ATOM	205	C	ALA A	24	1.531	45.479	31.893	1.00	31.41	A
ATOM	206	O	ALA A	24	0.562	46.183	31.608	1.00	31.49	A
ATOM	207	N	ARG A	25	2.428	45.825	32.816	1.00	30.94	A
ATOM	208	CA	ARG A	25	2.297	47.070	33.547	1.00	30.44	A
ATOM	209	CB	ARG A	25	3.197	47.066	34.798	1.00	32.01	A
ATOM	210	CG	ARG A	25	2.727	46.101	35.894	1.00	34.49	A
ATOM	211	CD	ARG A	25	3.471	46.326	37.218	1.00	39.65	A
ATOM	212	NE	ARG A	25	4.873	45.907	37.177	1.00	40.74	A
ATOM	213	CZ	ARG A	25	5.308	44.687	37.496	1.00	43.06	A
ATOM	214	NH1	ARG A	25	4.453	43.749	37.885	1.00	39.85	A
ATOM	215	NH2	ARG A	25	6.606	44.399	37.399	1.00	40.30	A
ATOM	216	C	ARG A	25	2.590	48.270	32.651	1.00	28.86	A
ATOM	217	O	ARG A	25	1.907	49.296	32.728	1.00	29.35	A
ATOM	218	N	ILE A	26	3.587	48.147	31.790	1.00	26.96	A
ATOM	219	CA	ILE A	26	3.917	49.226	30.875	1.00	29.07	A
ATOM	220	CB	ILE A	26	5.132	48.832	29.990	1.00	28.43	A
ATOM	221	CG2	ILE A	26	5.239	49.760	28.799	1.00	25.38	A
ATOM	222	CG1	ILE A	26	6.414	48.835	30.839	1.00	28.70	A
ATOM	223	CD1	ILE A	26	7.646	48.257	30.132	1.00	27.77	A
ATOM	224	C	ILE A	26	2.719	49.571	29.968	1.00	30.92	A
ATOM	225	O	ILE A	26	2.435	50.746	29.690	1.00	32.33	A
ATOM	226	N	LYS A	27	2.019	48.540	29.512	1.00	30.36	A
ATOM	227	CA	LYS A	27	0.887	48.730	28.627	1.00	30.40	A
ATOM	228	CB	LYS A	27	0.449	47.388	28.045	1.00	33.83	A
ATOM	229	CG	LYS A	27	1.520	46.729	27.185	1.00	39.64	A
ATOM	230	CD	LYS A	27	1.167	45.294	26.831	1.00	44.41	A
ATOM	231	CE	LYS A	27	-0.086	45.204	26.003	1.00	46.84	A

Figure 11D

ATOM	232	NZ	LYS	A	27	-0.384	43.774	25.698	1.00	53.94	A
ATOM	233	C	LYS	A	27	-0.267	49.402	29.344	1.00	28.67	A
ATOM	234	O	LYS	A	27	-0.919	50.252	28.767	1.00	26.05	A
ATOM	235	N	LYS	A	28	-0.511	49.020	30.593	1.00	27.68	A
ATOM	236	CA	LYS	A	28	-1.597	49.609	31.371	1.00	27.30	A
ATOM	237	CB	LYS	A	28	-1.797	48.845	32.691	1.00	24.82	A
ATOM	238	CG	LYS	A	28	-2.961	49.384	33.573	1.00	27.48	A
ATOM	239	CD	LYS	A	28	-4.263	49.506	32.744	1.00	31.59	A
ATOM	240	CE	LYS	A	28	-5.526	49.699	33.606	1.00	30.02	A
ATOM	241	NZ	LYS	A	28	-5.440	50.820	34.586	1.00	31.11	A
ATOM	242	C	LYS	A	28	-1.284	51.076	31.641	1.00	29.57	A
ATOM	243	O	LYS	A	28	-2.164	51.951	31.566	1.00	28.21	A
ATOM	244	N	LEU	A	29	-0.017	51.359	31.923	1.00	29.36	A
ATOM	245	CA	LEU	A	29	0.385	52.723	32.179	1.00	33.70	A
ATOM	246	CB	LEU	A	29	1.822	52.745	32.692	1.00	35.26	A
ATOM	247	CG	LEU	A	29	2.023	53.727	33.847	1.00	38.04	A
ATOM	248	CD1	LEU	A	29	3.363	53.485	34.506	1.00	39.85	A
ATOM	249	CD2	LEU	A	29	1.891	55.149	33.332	1.00	38.01	A
ATOM	250	C	LEU	A	29	0.243	53.561	30.905	1.00	34.59	A
ATOM	251	O	LEU	A	29	-0.281	54.691	30.927	1.00	37.16	A
ATOM	252	N	LEU	A	30	0.721	53.020	29.792	1.00	34.03	A
ATOM	253	CA	LEU	A	30	0.616	53.724	28.528	1.00	35.56	A
ATOM	254	CB	LEU	A	30	1.230	52.874	27.414	1.00	38.09	A
ATOM	255	CG	LEU	A	30	1.470	53.508	26.050	1.00	40.19	A
ATOM	256	CD1	LEU	A	30	2.270	54.805	26.163	1.00	39.79	A
ATOM	257	CD2	LEU	A	30	2.215	52.484	25.198	1.00	45.44	A
ATOM	258	C	LEU	A	30	-0.882	53.980	28.263	1.00	34.76	A
ATOM	259	O	LEU	A	30	-1.269	55.050	27.794	1.00	33.56	A
ATOM	260	N	GLN	A	31	-1.713	52.996	28.572	1.00	30.55	A
ATOM	261	CA	GLN	A	31	-3.152	53.142	28.401	1.00	31.04	A
ATOM	262	CB	GLN	A	31	-3.865	51.839	28.782	1.00	33.01	A
ATOM	263	CG	GLN	A	31	-5.397	51.924	28.839	1.00	37.09	A
ATOM	264	CD	GLN	A	31	-6.045	50.582	29.159	1.00	45.53	A
ATOM	265	OE1	GLN	A	31	-5.715	49.940	30.159	1.00	52.72	A
ATOM	266	NE2	GLN	A	31	-6.973	50.151	28.310	1.00	46.91	A
ATOM	267	C	GLN	A	31	-3.633	54.303	29.273	1.00	31.34	A
ATOM	268	O	GLN	A	31	-4.419	55.125	28.832	1.00	28.45	A
ATOM	269	N	LEU	A	32	-3.141	54.376	30.509	1.00	30.93	A
ATOM	270	CA	LEU	A	32	-3.523	55.459	31.393	1.00	30.83	A
ATOM	271	CB	LEU	A	32	-2.988	55.237	32.811	1.00	29.49	A
ATOM	272	CG	LEU	A	32	-3.572	54.156	33.732	1.00	31.79	A
ATOM	273	CD1	LEU	A	32	-2.810	54.215	35.075	1.00	33.29	A
ATOM	274	CD2	LEU	A	32	-5.058	54.376	33.972	1.00	25.39	A
ATOM	275	C	LEU	A	32	-3.031	56.797	30.860	1.00	32.26	A
ATOM	276	O	LEU	A	32	-3.707	57.810	31.031	1.00	35.77	A
ATOM	277	N	THR	A	33	-1.872	56.798	30.198	1.00	31.70	A
ATOM	278	CA	THR	A	33	-1.298	58.019	29.640	1.00	33.33	A
ATOM	279	CB	THR	A	33	0.158	57.787	29.156	1.00	35.07	A
ATOM	280	OG1	THR	A	33	0.949	57.272	30.238	1.00	39.00	A
ATOM	281	CG2	THR	A	33	0.776	59.087	28.687	1.00	34.58	A
ATOM	282	C	THR	A	33	-2.120	58.560	28.471	1.00	33.63	A
ATOM	283	O	THR	A	33	-2.237	59.767	28.298	1.00	33.87	A
ATOM	284	N	VAL	A	34	-2.682	57.660	27.670	1.00	35.32	A
ATOM	285	CA	VAL	A	34	-3.507	58.046	26.531	1.00	36.90	A
ATOM	286	CB	VAL	A	34	-3.810	56.832	25.622	1.00	36.47	A
ATOM	287	CG1	VAL	A	34	-4.825	57.200	24.550	1.00	34.36	A
ATOM	288	CG2	VAL	A	34	-2.514	56.354	24.966	1.00	38.97	A
ATOM	289	C	VAL	A	34	-4.809	58.655	27.036	1.00	37.01	A
ATOM	290	O	VAL	A	34	-5.250	59.695	26.540	1.00	35.59	A
ATOM	291	N	TRP	A	35	-5.403	57.992	28.022	1.00	36.34	A

Figure 11E

ATOM	292	CA	TRP	A	35	-6.645	58.429	28.648	1.00	38.95	A
ATOM	293	CB	TRP	A	35	-7.022	57.429	29.742	1.00	44.03	A
ATOM	294	CG	TRP	A	35	-8.302	57.716	30.478	1.00	45.10	A
ATOM	295	CD2	TRP	A	35	-8.445	58.535	31.640	1.00	46.19	A
ATOM	296	CE2	TRP	A	35	-9.820	58.545	31.973	1.00	47.39	A
ATOM	297	CE3	TRP	A	35	-7.556	59.277	32.429	1.00	46.15	A
ATOM	298	CD1	TRP	A	35	-9.549	57.260	30.166	1.00	45.42	A
ATOM	299	NE1	TRP	A	35	-10.468	57.752	31.063	1.00	47.75	A
ATOM	300	CZ2	TRP	A	35	-10.317	59.258	33.067	1.00	48.12	A
ATOM	301	CZ3	TRP	A	35	-8.049	59.991	33.509	1.00	44.34	A
ATOM	302	CH2	TRP	A	35	-9.419	59.968	33.824	1.00	47.03	A
ATOM	303	C	TRP	A	35	-6.408	59.814	29.259	1.00	40.04	A
ATOM	304	O	TRP	A	35	-7.155	60.759	29.013	1.00	39.15	A
ATOM	305	N	GLY	A	36	-5.352	59.934	30.055	1.00	38.98	A
ATOM	306	CA	GLY	A	36	-5.039	61.211	30.658	1.00	38.44	A
ATOM	307	C	GLY	A	36	-5.034	62.327	29.634	1.00	38.41	A
ATOM	308	O	GLY	A	36	-5.626	63.390	29.845	1.00	40.58	A
ATOM	309	N	ILE	A	37	-4.356	62.094	28.517	1.00	39.01	A
ATOM	310	CA	ILE	A	37	-4.279	63.079	27.451	1.00	40.60	A
ATOM	311	CB	ILE	A	37	-3.395	62.584	26.301	1.00	40.20	A
ATOM	312	CG2	ILE	A	37	-3.509	63.517	25.136	1.00	39.97	A
ATOM	313	CG1	ILE	A	37	-1.939	62.477	26.767	1.00	41.25	A
ATOM	314	CD1	ILE	A	37	-1.036	61.777	25.778	1.00	38.31	A
ATOM	315	C	ILE	A	37	-5.662	63.366	26.886	1.00	42.00	A
ATOM	316	O	ILE	A	37	-6.019	64.516	26.654	1.00	42.52	A
ATOM	317	N	LYS	A	38	-6.438	62.317	26.660	1.00	42.56	A
ATOM	318	CA	LYS	A	38	-7.766	62.505	26.112	1.00	45.16	A
ATOM	319	CB	LYS	A	38	-8.459	61.156	25.925	1.00	46.50	A
ATOM	320	CG	LYS	A	38	-9.683	61.235	25.026	1.00	53.52	A
ATOM	321	CD	LYS	A	38	-10.840	62.017	25.651	1.00	55.55	A
ATOM	322	CE	LYS	A	38	-11.812	62.480	24.581	1.00	56.01	A
ATOM	323	NZ	LYS	A	38	-11.165	63.504	23.714	1.00	55.27	A
ATOM	324	C	LYS	A	38	-8.594	63.405	27.025	1.00	46.34	A
ATOM	325	O	LYS	A	38	-9.237	64.343	26.561	1.00	48.52	A
ATOM	326	N	GLN	A	39	-8.554	63.120	28.322	1.00	47.82	A
ATOM	327	CA	GLN	A	39	-9.303	63.877	29.318	1.00	49.21	A
ATOM	328	CB	GLN	A	39	-9.142	63.230	30.691	1.00	52.07	A
ATOM	329	CG	GLN	A	39	-9.431	61.742	30.727	1.00	59.01	A
ATOM	330	CD	GLN	A	39	-10.889	61.409	30.513	1.00	61.01	A
ATOM	331	OE1	GLN	A	39	-11.742	61.800	31.310	1.00	63.56	A
ATOM	332	NE2	GLN	A	39	-11.188	60.677	29.437	1.00	62.00	A
ATOM	333	C	GLN	A	39	-8.840	65.324	29.412	1.00	48.78	A
ATOM	334	O	GLN	A	39	-9.649	66.243	29.431	1.00	48.03	A
ATOM	335	N	LEU	A	40	-7.530	65.522	29.472	1.00	49.67	A
ATOM	336	CA	LEU	A	40	-6.980	66.861	29.590	1.00	50.78	A
ATOM	337	CB	LEU	A	40	-5.479	66.785	29.868	1.00	49.62	A
ATOM	338	CG	LEU	A	40	-4.736	68.118	29.982	1.00	47.99	A
ATOM	339	CD1	LEU	A	40	-5.416	69.030	31.011	1.00	51.32	A
ATOM	340	CD2	LEU	A	40	-3.300	67.852	30.376	1.00	48.82	A
ATOM	341	C	LEU	A	40	-7.227	67.736	28.363	1.00	53.20	A
ATOM	342	O	LEU	A	40	-7.230	68.964	28.457	1.00	53.67	A
ATOM	343	N	GLN	A	41	-7.433	67.104	27.215	1.00	56.61	A
ATOM	344	CA	GLN	A	41	-7.649	67.850	25.994	1.00	60.81	A
ATOM	345	CB	GLN	A	41	-7.295	66.994	24.781	1.00	60.00	A
ATOM	346	CG	GLN	A	41	-7.257	67.753	23.467	1.00	61.60	A
ATOM	347	CD	GLN	A	41	-6.756	66.885	22.330	1.00	61.14	A
ATOM	348	OE1	GLN	A	41	-5.630	66.377	22.367	1.00	56.12	A
ATOM	349	NE2	GLN	A	41	-7.598	66.697	21.316	1.00	60.61	A
ATOM	350	C	GLN	A	41	-9.084	68.344	25.915	1.00	63.54	A
ATOM	351	O	GLN	A	41	-9.388	69.277	25.179	1.00	65.13	A

Figure 11F

ATOM	352	N	ALA A	42	-9.971	67.722	26.679	1.00 67.16	A
ATOM	353	CA	ALA A	42	-11.362	68.150	26.693	1.00 70.08	A
ATOM	354	CB	ALA A	42	-12.252	67.043	27.249	1.00 68.59	A
ATOM	355	C	ALA A	42	-11.461	69.423	27.556	1.00 72.76	A
ATOM	356	O	ALA A	42	-12.506	69.748	28.123	1.00 73.45	A
ATOM	357	N	ARG A	43	-10.338	70.137	27.642	1.00 75.35	A
ATOM	358	CA	ARG A	43	-10.202	71.377	28.413	1.00 76.97	A
ATOM	359	CB	ARG A	43	-9.391	71.131	29.705	1.00 77.23	A
ATOM	360	CG	ARG A	43	-10.130	70.250	30.753	1.00 77.83	A
ATOM	361	CD	ARG A	43	-9.265	69.690	31.889	1.00 76.18	A
ATOM	362	NE	ARG A	43	-10.053	68.919	32.864	1.00 76.19	A
ATOM	363	CZ	ARG A	43	-10.933	67.967	32.551	1.00 76.17	A
ATOM	364	NH1	ARG A	43	-11.153	67.657	31.284	1.00 76.24	A
ATOM	365	NH2	ARG A	43	-11.605	67.326	33.507	1.00 77.89	A
ATOM	366	C	ARG A	43	-9.560	72.481	27.570	1.00 79.19	A
ATOM	367	O	ARG A	43	-10.131	72.882	26.548	1.00 79.42	A
ATOM	368	N	ILE A	44	-8.381	72.970	27.993	1.00 81.42	A
ATOM	369	CA	ILE A	44	-7.646	74.059	27.276	1.00 84.32	A
ATOM	370	CB	ILE A	44	-6.073	73.998	27.495	1.00 84.97	A
ATOM	371	CG2	ILE A	44	-5.292	74.824	26.419	1.00 85.80	A
ATOM	372	CG1	ILE A	44	-5.728	74.612	28.829	1.00 85.52	A
ATOM	373	CD1	ILE A	44	-6.344	76.011	29.055	1.00 87.04	A
ATOM	374	C	ILE A	44	-7.908	73.987	25.790	1.00 86.80	A
ATOM	375	O	ILE A	44	-8.577	74.829	25.234	1.00 87.60	A
ATOM	376	N	LEU A	45	-7.318	73.007	25.145	1.00 87.99	A
ATOM	377	CA	LEU A	45	-7.541	72.910	23.737	1.00 88.13	A
ATOM	378	CB	LEU A	45	-6.257	72.509	23.009	1.00 88.79	A
ATOM	379	CG	LEU A	45	-5.940	73.339	21.770	1.00 90.46	A
ATOM	380	CD1	LEU A	45	-7.147	73.370	20.837	1.00 91.58	A
ATOM	381	CD2	LEU A	45	-5.596	74.779	22.173	1.00 90.84	A
ATOM	382	C	LEU A	45	-8.656	71.944	23.376	1.00 88.30	A
ATOM	383	O	LEU A	45	-9.507	71.665	24.291	1.00 87.82	A
ATOM	384	NT	LEU A	45	-8.614	71.561	22.151	1.00 88.77	A
ATOM	385	CA	ACE B	0	29.175	18.175	21.874	1.00 35.90	B
ATOM	386	C	ACE B	0	27.867	18.849	22.146	1.00 36.69	B
ATOM	387	O	ACE B	0	27.836	20.078	22.299	1.00 33.24	B
ATOM	388	N	ARG B	1	26.771	18.065	22.218	1.00 32.69	B
ATOM	389	CA	ARG B	1	25.440	18.590	22.450	1.00 34.24	B
ATOM	390	CB	ARG B	1	24.436	17.446	22.644	1.00 33.49	B
ATOM	391	CG	ARG B	1	22.976	17.878	22.651	1.00 32.92	B
ATOM	392	CD	ARG B	1	22.436	18.177	21.260	1.00 34.95	B
ATOM	393	NE	ARG B	1	22.366	16.972	20.443	1.00 38.88	B
ATOM	394	CZ	ARG B	1	21.548	15.952	20.706	1.00 42.79	B
ATOM	395	NH1	ARG B	1	20.740	16.012	21.765	1.00 44.66	B
ATOM	396	NH2	ARG B	1	21.550	14.868	19.943	1.00 39.72	B
ATOM	397	C	ARG B	1	25.424	19.498	23.685	1.00 35.96	B
ATOM	398	O	ARG B	1	24.920	20.617	23.628	1.00 36.55	B
ATOM	399	N	MET B	2	26.008	19.009	24.779	1.00 39.89	B
ATOM	400	CA	MET B	2	26.077	19.769	26.022	1.00 43.08	B
ATOM	401	CB	MET B	2	27.113	19.163	26.972	1.00 43.87	B
ATOM	402	CG	MET B	2	26.728	17.847	27.623	1.00 46.86	B
ATOM	403	SD	MET B	2	25.304	18.010	28.700	1.00 52.01	B
ATOM	404	CE	MET B	2	24.024	18.375	27.524	1.00 52.70	B
ATOM	405	C	MET B	2	26.440	21.219	25.789	1.00 45.76	B
ATOM	406	O	MET B	2	25.723	22.121	26.212	1.00 44.09	B
ATOM	407	N	LYS B	3	27.570	21.414	25.125	1.00 47.94	B
ATOM	408	CA	LYS B	3	28.082	22.736	24.820	1.00 52.42	B
ATOM	409	CB	LYS B	3	29.455	22.565	24.151	1.00 54.64	B
ATOM	410	CG	LYS B	3	30.552	23.540	24.595	1.00 58.36	B
ATOM	411	CD	LYS B	3	30.382	24.937	24.030	1.00 60.17	B

Figure 11G

ATOM	412	CE	LYS	B	3	31.618	25.777	24.321	1.00 62.06	B
ATOM	413	NZ	LYS	B	3	31.561	27.140	23.704	1.00 63.71	B
ATOM	414	C	LYS	B	3	27.095	23.479	23.907	1.00 52.65	B
ATOM	415	O	LYS	B	3	26.858	24.671	24.092	1.00 52.44	B
ATOM	416	N	GLN	B	4	26.517	22.774	22.934	1.00 52.13	B
ATOM	417	CA	GLN	B	4	25.549	23.387	22.032	1.00 54.04	B
ATOM	418	CB	GLN	B	4	24.930	22.330	21.105	1.00 57.72	B
ATOM	419	CG	GLN	B	4	25.792	21.880	19.925	1.00 60.44	B
ATOM	420	CD	GLN	B	4	25.855	22.923	18.816	1.00 62.71	B
ATOM	421	OE1	GLN	B	4	26.404	24.017	18.997	1.00 64.51	B
ATOM	422	NE2	GLN	B	4	25.276	22.592	17.661	1.00 62.62	B
ATOM	423	C	GLN	B	4	24.441	24.062	22.836	1.00 52.63	B
ATOM	424	O	GLN	B	4	24.013	25.162	22.518	1.00 53.56	B
ATOM	425	N	ILE	B	5	23.982	23.379	23.878	1.00 52.62	B
ATOM	426	CA	ILE	B	5	22.929	23.880	24.758	1.00 52.43	B
ATOM	427	CB	ILE	B	5	22.443	22.766	25.721	1.00 51.17	B
ATOM	428	CG2	ILE	B	5	21.412	23.329	26.691	1.00 52.10	B
ATOM	429	CG1	ILE	B	5	21.871	21.592	24.917	1.00 52.55	B
ATOM	430	CD1	ILE	B	5	21.496	20.363	25.754	1.00 53.47	B
ATOM	431	C	ILE	B	5	23.452	25.043	25.600	1.00 53.54	B
ATOM	432	O	ILE	B	5	22.743	26.013	25.849	1.00 52.58	B
ATOM	433	N	GLU	B	6	24.701	24.932	26.036	1.00 55.54	B
ATOM	434	CA	GLU	B	6	25.309	25.970	26.850	1.00 56.11	B
ATOM	435	CB	GLU	B	6	26.637	25.477	27.437	1.00 53.75	B
ATOM	436	CG	GLU	B	6	26.487	24.157	28.171	1.00 53.07	B
ATOM	437	CD	GLU	B	6	27.729	23.735	28.939	1.00 50.56	B
ATOM	438	OE1	GLU	B	6	28.816	23.611	28.329	1.00 49.24	B
ATOM	439	OE2	GLU	B	6	27.604	23.516	30.159	1.00 47.31	B
ATOM	440	C	GLU	B	6	25.522	27.217	26.009	1.00 57.04	B
ATOM	441	O	GLU	B	6	25.418	28.335	26.515	1.00 58.94	B
ATOM	442	N	ASP	B	7	25.811	27.031	24.725	1.00 57.18	B
ATOM	443	CA	ASP	B	7	26.003	28.179	23.848	1.00 58.51	B
ATOM	444	CB	ASP	B	7	26.681	27.772	22.536	1.00 59.88	B
ATOM	445	CG	ASP	B	7	28.121	27.339	22.732	1.00 62.42	B
ATOM	446	OD1	ASP	B	7	28.827	27.979	23.542	1.00 62.53	B
ATOM	447	OD2	ASP	B	7	28.559	26.382	22.056	1.00 66.19	B
ATOM	448	C	ASP	B	7	24.668	28.858	23.543	1.00 58.25	B
ATOM	449	O	ASP	B	7	24.624	30.070	23.314	1.00 56.00	B
ATOM	450	N	LYS	B	8	23.591	28.069	23.547	1.00 57.96	B
ATOM	451	CA	LYS	B	8	22.240	28.563	23.276	1.00 57.58	B
ATOM	452	CB	LYS	B	8	21.331	27.405	22.838	1.00 57.99	B
ATOM	453	CG	LYS	B	8	19.911	27.844	22.484	1.00 60.08	B
ATOM	454	CD	LYS	B	8	19.915	28.785	21.280	1.00 60.12	B
ATOM	455	CE	LYS	B	8	18.697	29.725	21.268	1.00 60.76	B
ATOM	456	NZ	LYS	B	8	17.371	29.062	21.146	1.00 58.46	B
ATOM	457	C	LYS	B	8	21.653	29.248	24.517	1.00 56.86	B
ATOM	458	O	LYS	B	8	20.832	30.166	24.411	1.00 53.70	B
ATOM	459	N	ILE	B	9	22.077	28.790	25.689	1.00 57.87	B
ATOM	460	CA	ILE	B	9	21.621	29.368	26.947	1.00 59.31	B
ATOM	461	CB	ILE	B	9	22.073	28.517	28.161	1.00 57.40	B
ATOM	462	CG2	ILE	B	9	21.788	29.270	29.459	1.00 57.21	B
ATOM	463	CG1	ILE	B	9	21.361	27.165	28.154	1.00 56.21	B
ATOM	464	CD1	ILE	B	9	21.885	26.199	29.212	1.00 54.49	B
ATOM	465	C	ILE	B	9	22.216	30.770	27.093	1.00 60.74	B
ATOM	466	O	ILE	B	9	21.565	31.682	27.608	1.00 61.51	B
ATOM	467	N	GLU	B	10	23.456	30.923	26.633	1.00 61.69	B
ATOM	468	CA	GLU	B	10	24.170	32.198	26.691	1.00 63.76	B
ATOM	469	CB	GLU	B	10	25.629	32.000	26.279	1.00 63.63	B
ATOM	470	CG	GLU	B	10	26.456	33.275	26.254	1.00 65.58	B
ATOM	471	CD	GLU	B	10	27.854	33.054	25.707	1.00 66.48	B

Figure 11H

ATOM	472	OE1	GLU	B	10	27.979	32.751	24.499	1.00	67.38	B
ATOM	473	OE2	GLU	B	10	28.824	33.173	26.485	1.00	66.28	B
ATOM	474	C	GLU	B	10	23.515	33.211	25.757	1.00	65.16	B
ATOM	475	O	GLU	B	10	23.261	34.351	26.141	1.00	65.81	B
ATOM	476	N	GLU	B	11	23.255	32.785	24.524	1.00	66.64	B
ATOM	477	CA	GLU	B	11	22.617	33.637	23.529	1.00	67.59	B
ATOM	478	CB	GLU	B	11	22.348	32.832	22.252	1.00	68.72	B
ATOM	479	CG	GLU	B	11	21.735	33.636	21.117	1.00	72.88	B
ATOM	480	CD	GLU	B	11	22.556	34.864	20.767	1.00	74.80	B
ATOM	481	OE1	GLU	B	11	23.775	34.717	20.526	1.00	75.81	B
ATOM	482	OE2	GLU	B	11	21.978	35.975	20.731	1.00	74.99	B
ATOM	483	C	GLU	B	11	21.307	34.197	24.098	1.00	67.17	B
ATOM	484	O	GLU	B	11	20.998	35.381	23.918	1.00	68.06	B
ATOM	485	N	ILE	B	12	20.541	33.348	24.784	1.00	64.61	B
ATOM	486	CA	ILE	B	12	19.288	33.790	25.389	1.00	61.65	B
ATOM	487	CB	ILE	B	12	18.458	32.600	25.926	1.00	62.84	B
ATOM	488	CG2	ILE	B	12	17.416	33.094	26.940	1.00	62.63	B
ATOM	489	CG1	ILE	B	12	17.799	31.864	24.750	1.00	62.13	B
ATOM	490	CD1	ILE	B	12	16.910	30.698	25.156	1.00	61.39	B
ATOM	491	C	ILE	B	12	19.553	34.776	26.522	1.00	58.17	B
ATOM	492	O	ILE	B	12	19.010	35.881	26.523	1.00	55.05	B
ATOM	493	N	GLU	B	13	20.388	34.384	27.479	1.00	55.87	B
ATOM	494	CA	GLU	B	13	20.710	35.268	28.600	1.00	54.71	B
ATOM	495	CB	GLU	B	13	21.817	34.669	29.477	1.00	50.19	B
ATOM	496	CG	GLU	B	13	21.447	33.331	30.109	1.00	49.30	B
ATOM	497	CD	GLU	B	13	22.577	32.729	30.933	1.00	49.10	B
ATOM	498	OE1	GLU	B	13	23.741	32.765	30.472	1.00	50.79	B
ATOM	499	OE2	GLU	B	13	22.304	32.194	32.027	1.00	47.00	B
ATOM	500	C	GLU	B	13	21.166	36.612	28.047	1.00	55.57	B
ATOM	501	O	GLU	B	13	20.790	37.667	28.557	1.00	56.33	B
ATOM	502	N	SER	B	14	21.950	36.559	26.977	1.00	56.02	B
ATOM	503	CA	SER	B	14	22.468	37.763	26.350	1.00	55.71	B
ATOM	504	CB	SER	B	14	23.488	37.389	25.278	1.00	54.62	B
ATOM	505	OG	SER	B	14	23.968	38.550	24.629	1.00	56.74	B
ATOM	506	C	SER	B	14	21.366	38.624	25.736	1.00	55.96	B
ATOM	507	O	SER	B	14	21.469	39.854	25.696	1.00	54.91	B
ATOM	508	N	LYS	B	15	20.310	37.979	25.263	1.00	55.94	B
ATOM	509	CA	LYS	B	15	19.208	38.704	24.650	1.00	56.72	B
ATOM	510	CB	LYS	B	15	18.454	37.779	23.693	1.00	55.67	B
ATOM	511	CG	LYS	B	15	17.494	38.484	22.772	1.00	58.33	B
ATOM	512	CD	LYS	B	15	17.000	37.527	21.705	1.00	59.89	B
ATOM	513	CE	LYS	B	15	16.440	38.282	20.518	1.00	60.44	B
ATOM	514	NZ	LYS	B	15	16.020	37.375	19.412	1.00	63.67	B
ATOM	515	C	LYS	B	15	18.282	39.207	25.748	1.00	56.31	B
ATOM	516	O	LYS	B	15	17.716	40.296	25.661	1.00	56.65	B
ATOM	517	N	GLN	B	16	18.146	38.403	26.791	1.00	56.76	B
ATOM	518	CA	GLN	B	16	17.293	38.748	27.911	1.00	57.28	B
ATOM	519	CB	GLN	B	16	17.306	37.604	28.923	1.00	56.94	B
ATOM	520	CG	GLN	B	16	16.000	37.394	29.652	1.00	55.90	B
ATOM	521	CD	GLN	B	16	15.908	36.017	30.300	1.00	56.24	B
ATOM	522	OE1	GLN	B	16	16.613	35.722	31.263	1.00	57.78	B
ATOM	523	NE2	GLN	B	16	15.044	35.160	29.760	1.00	55.69	B
ATOM	524	C	GLN	B	16	17.825	40.040	28.528	1.00	58.82	B
ATOM	525	O	GLN	B	16	17.049	40.929	28.905	1.00	59.68	B
ATOM	526	N	LYS	B	17	19.148	40.163	28.621	1.00	59.44	B
ATOM	527	CA	LYS	B	17	19.711	41.379	29.189	1.00	59.84	B
ATOM	528	CB	LYS	B	17	21.228	41.275	29.386	1.00	60.80	B
ATOM	529	CG	LYS	B	17	21.740	42.343	30.356	1.00	64.52	B
ATOM	530	CD	LYS	B	17	23.250	42.325	30.576	1.00	65.30	B
ATOM	531	CE	LYS	B	17	24.008	42.784	29.344	1.00	67.22	B

Figure III

ATOM	532	NZ	LYS	B	17	25.465	42.963	29.625	1.00	67.09	B
ATOM	533	C	LYS	B	17	19.389	42.522	28.230	1.00	59.16	B
ATOM	534	O	LYS	B	17	19.088	43.634	28.656	1.00	55.77	B
ATOM	535	N	LYS	B	18	19.433	42.233	26.931	1.00	58.38	B
ATOM	536	CA	LYS	B	18	19.128	43.248	25.931	1.00	58.35	B
ATOM	537	CB	LYS	B	18	19.247	42.675	24.511	1.00	59.38	B
ATOM	538	CG	LYS	B	18	20.617	42.083	24.130	1.00	61.47	B
ATOM	539	CD	LYS	B	18	21.768	43.111	24.099	1.00	61.91	B
ATOM	540	CE	LYS	B	18	22.034	43.761	25.461	1.00	63.50	B
ATOM	541	NZ	LYS	B	18	23.248	44.620	25.423	1.00	63.66	B
ATOM	542	C	LYS	B	18	17.706	43.761	26.163	1.00	58.27	B
ATOM	543	O	LYS	B	18	17.475	44.969	26.254	1.00	58.82	B
ATOM	544	N	ILE	B	19	16.757	42.835	26.268	1.00	56.89	B
ATOM	545	CA	ILE	B	19	15.356	43.189	26.488	1.00	53.76	B
ATOM	546	CB	ILE	B	19	14.455	41.931	26.488	1.00	53.33	B
ATOM	547	CG2	ILE	B	19	13.057	42.286	26.976	1.00	52.66	B
ATOM	548	CG1	ILE	B	19	14.416	41.322	25.081	1.00	52.79	B
ATOM	549	CD1	ILE	B	19	13.543	40.069	24.970	1.00	54.45	B
ATOM	550	C	ILE	B	19	15.117	43.961	27.786	1.00	52.88	B
ATOM	551	O	ILE	B	19	14.327	44.897	27.809	1.00	51.74	B
ATOM	552	N	GLU	B	20	15.781	43.565	28.869	1.00	51.04	B
ATOM	553	CA	GLU	B	20	15.601	44.267	30.128	1.00	50.08	B
ATOM	554	CB	GLU	B	20	16.403	43.613	31.253	1.00	49.90	B
ATOM	555	CG	GLU	B	20	15.969	42.207	31.584	1.00	54.19	B
ATOM	556	CD	GLU	B	20	16.761	41.620	32.736	1.00	55.98	B
ATOM	557	OE1	GLU	B	20	18.010	41.568	32.641	1.00	53.23	B
ATOM	558	OE2	GLU	B	20	16.127	41.215	33.735	1.00	56.20	B
ATOM	559	C	GLU	B	20	16.053	45.706	29.965	1.00	49.26	B
ATOM	560	O	GLU	B	20	15.479	46.611	30.561	1.00	48.88	B
ATOM	561	N	ASN	B	21	17.093	45.912	29.163	1.00	49.15	B
ATOM	562	CA	ASN	B	21	17.596	47.256	28.930	1.00	49.99	B
ATOM	563	CB	ASN	B	21	18.885	47.229	28.098	1.00	51.35	B
ATOM	564	CG	ASN	B	21	20.054	46.576	28.834	1.00	54.79	B
ATOM	565	OD1	ASN	B	21	20.421	46.978	29.943	1.00	55.96	B
ATOM	566	ND2	ASN	B	21	20.656	45.572	28.205	1.00	57.15	B
ATOM	567	C	ASN	B	21	16.537	48.078	28.202	1.00	49.83	B
ATOM	568	O	ASN	B	21	16.249	49.209	28.591	1.00	50.14	B
ATOM	569	N	GLU	B	22	15.957	47.497	27.153	1.00	47.34	B
ATOM	570	CA	GLU	B	22	14.942	48.160	26.354	1.00	44.99	B
ATOM	571	CB	GLU	B	22	14.534	47.272	25.174	1.00	44.99	B
ATOM	572	CG	GLU	B	22	13.703	47.990	24.116	1.00	51.85	B
ATOM	573	CD	GLU	B	22	14.377	49.268	23.621	1.00	54.71	B
ATOM	574	OE1	GLU	B	22	15.543	49.191	23.182	1.00	55.60	B
ATOM	575	OE2	GLU	B	22	13.743	50.350	23.673	1.00	57.01	B
ATOM	576	C	GLU	B	22	13.710	48.521	27.183	1.00	44.17	B
ATOM	577	O	GLU	B	22	13.044	49.527	26.916	1.00	45.50	B
ATOM	578	N	ILE	B	23	13.386	47.693	28.169	1.00	42.28	B
ATOM	579	CA	ILE	B	23	12.241	47.977	29.024	1.00	40.61	B
ATOM	580	CB	ILE	B	23	11.801	46.724	29.809	1.00	38.57	B
ATOM	581	CG2	ILE	B	23	10.836	47.096	30.925	1.00	37.31	B
ATOM	582	CG1	ILE	B	23	11.138	45.733	28.850	1.00	38.28	B
ATOM	583	CD1	ILE	B	23	10.634	44.436	29.530	1.00	38.32	B
ATOM	584	C	ILE	B	23	12.626	49.108	29.974	1.00	41.50	B
ATOM	585	O	ILE	B	23	11.793	49.926	30.349	1.00	41.54	B
ATOM	586	N	ALA	B	24	13.898	49.170	30.348	1.00	40.42	B
ATOM	587	CA	ALA	B	24	14.349	50.240	31.224	1.00	38.49	B
ATOM	588	CB	ALA	B	24	15.811	50.059	31.578	1.00	34.26	B
ATOM	589	C	ALA	B	24	14.147	51.562	30.490	1.00	37.76	B
ATOM	590	O	ALA	B	24	13.674	52.528	31.078	1.00	38.39	B
ATOM	591	N	ARG	B	25	14.498	51.591	29.204	1.00	36.47	B

Figure 11J

ATOM	592	CA	ARG	B	25	14.354	52.796	28.394	1.00	38.10	B
ATOM	593	CB	ARG	B	25	15.086	52.644	27.051	1.00	40.70	B
ATOM	594	CG	ARG	B	25	16.609	52.668	27.195	1.00	46.74	B
ATOM	595	CD	ARG	B	25	17.315	52.949	25.879	1.00	51.86	B
ATOM	596	NE	ARG	B	25	17.268	51.823	24.954	1.00	56.83	B
ATOM	597	CZ	ARG	B	25	17.894	50.666	25.152	1.00	59.56	B
ATOM	598	NH1	ARG	B	25	18.615	50.477	26.253	1.00	60.08	B
ATOM	599	NH2	ARG	B	25	17.792	49.696	24.257	1.00	59.81	B
ATOM	600	C	ARG	B	25	12.901	53.185	28.158	1.00	36.71	B
ATOM	601	O	ARG	B	25	12.555	54.361	28.165	1.00	36.54	B
ATOM	602	N	ILE	B	26	12.051	52.197	27.942	1.00	36.23	B
ATOM	603	CA	ILE	B	26	10.642	52.454	27.733	1.00	34.33	B
ATOM	604	CB	ILE	B	26	9.944	51.152	27.370	1.00	34.16	B
ATOM	605	CG2	ILE	B	26	8.432	51.293	27.496	1.00	31.45	B
ATOM	606	CG1	ILE	B	26	10.423	50.722	25.985	1.00	34.01	B
ATOM	607	CD1	ILE	B	26	9.879	49.403	25.540	1.00	34.37	B
ATOM	608	C	ILE	B	26	10.046	53.059	29.005	1.00	34.32	B
ATOM	609	O	ILE	B	26	9.317	54.053	28.956	1.00	33.13	B
ATOM	610	N	LYS	B	27	10.371	52.457	30.141	1.00	34.59	B
ATOM	611	CA	LYS	B	27	9.898	52.941	31.433	1.00	35.31	B
ATOM	612	CB	LYS	B	27	10.366	52.005	32.544	1.00	36.43	B
ATOM	613	CG	LYS	B	27	9.398	50.872	32.885	1.00	40.24	B
ATOM	614	CD	LYS	B	27	10.162	49.643	33.347	1.00	44.60	B
ATOM	615	CE	LYS	B	27	11.278	49.991	34.334	1.00	50.65	B
ATOM	616	NZ	LYS	B	27	12.209	48.831	34.560	1.00	54.97	B
ATOM	617	C	LYS	B	27	10.382	54.355	31.712	1.00	35.58	B
ATOM	618	O	LYS	B	27	9.666	55.140	32.318	1.00	36.82	B
ATOM	619	N	LYS	B	28	11.599	54.670	31.268	1.00	36.91	B
ATOM	620	CA	LYS	B	28	12.189	55.993	31.463	1.00	37.71	B
ATOM	621	CB	LYS	B	28	13.627	56.017	30.958	1.00	42.60	B
ATOM	622	CG	LYS	B	28	14.604	56.755	31.851	1.00	49.26	B
ATOM	623	CD	LYS	B	28	15.299	55.778	32.818	1.00	55.52	B
ATOM	624	CE	LYS	B	28	14.318	54.979	33.680	1.00	58.79	B
ATOM	625	NZ	LYS	B	28	15.015	53.887	34.421	1.00	59.10	B
ATOM	626	C	LYS	B	28	11.397	57.044	30.677	1.00	37.60	B
ATOM	627	O	LYS	B	28	10.956	58.045	31.240	1.00	40.12	B
ATOM	628	N	LEU	B	29	11.250	56.826	29.368	1.00	35.33	B
ATOM	629	CA	LEU	B	29	10.515	57.754	28.524	1.00	35.90	B
ATOM	630	CB	LEU	B	29	10.440	57.267	27.071	1.00	36.49	B
ATOM	631	CG	LEU	B	29	9.495	58.127	26.202	1.00	37.58	B
ATOM	632	CD1	LEU	B	29	9.958	59.581	26.260	1.00	36.39	B
ATOM	633	CD2	LEU	B	29	9.441	57.641	24.744	1.00	35.00	B
ATOM	634	C	LEU	B	29	9.103	57.912	29.047	1.00	35.09	B
ATOM	635	O	LEU	B	29	8.568	59.015	29.095	1.00	34.76	B
ATOM	636	N	LEU	B	30	8.512	56.787	29.426	1.00	33.74	B
ATOM	637	CA	LEU	B	30	7.161	56.746	29.946	1.00	30.65	B
ATOM	638	CB	LEU	B	30	6.789	55.294	30.181	1.00	32.72	B
ATOM	639	CG	LEU	B	30	5.385	54.822	30.558	1.00	31.65	B
ATOM	640	CD1	LEU	B	30	4.353	55.404	29.599	1.00	34.37	B
ATOM	641	CD2	LEU	B	30	5.377	53.282	30.511	1.00	31.69	B
ATOM	642	C	LEU	B	30	6.985	57.588	31.213	1.00	31.56	B
ATOM	643	O	LEU	B	30	6.051	58.398	31.301	1.00	26.54	B
ATOM	644	N	GLN	B	31	7.860	57.442	32.206	1.00	31.24	B
ATOM	645	CA	GLN	B	31	7.668	58.265	33.398	1.00	33.01	B
ATOM	646	CB	GLN	B	31	8.551	57.801	34.564	1.00	33.79	B
ATOM	647	CG	GLN	B	31	10.013	57.729	34.321	1.00	40.81	B
ATOM	648	CD	GLN	B	31	10.737	57.086	35.491	1.00	44.04	B
ATOM	649	OE1	GLN	B	31	10.804	57.648	36.598	1.00	43.99	B
ATOM	650	NE2	GLN	B	31	11.270	55.889	35.258	1.00	41.97	B
ATOM	651	C	GLN	B	31	7.906	59.734	33.072	1.00	34.12	B

Figure 11K

ATOM	652	O	GLN	B	31	7.420	60.636	33.766	1.00	30.63	B
ATOM	653	N	LEU	B	32	8.629	59.961	31.984	1.00	34.46	B
ATOM	654	CA	LEU	B	32	8.935	61.292	31.523	1.00	36.10	B
ATOM	655	CB	LEU	B	32	10.070	61.231	30.504	1.00	40.01	B
ATOM	656	CG	LEU	B	32	10.340	62.546	29.775	1.00	40.15	B
ATOM	657	CD1	LEU	B	32	10.853	63.586	30.765	1.00	43.23	B
ATOM	658	CD2	LEU	B	32	11.354	62.310	28.668	1.00	43.00	B
ATOM	659	C	LEU	B	32	7.711	61.949	30.890	1.00	36.08	B
ATOM	660	O	LEU	B	32	7.552	63.162	30.964	1.00	37.71	B
ATOM	661	N	THR	B	33	6.859	61.149	30.255	1.00	32.40	B
ATOM	662	CA	THR	B	33	5.659	61.679	29.617	1.00	31.31	B
ATOM	663	CB	THR	B	33	5.179	60.753	28.480	1.00	30.70	B
ATOM	664	OG1	THR	B	33	4.536	59.603	29.030	1.00	40.03	B
ATOM	665	CG2	THR	B	33	6.371	60.282	27.654	1.00	31.28	B
ATOM	666	C	THR	B	33	4.550	61.845	30.668	1.00	30.03	B
ATOM	667	O	THR	B	33	3.739	62.772	30.585	1.00	30.10	B
ATOM	668	N	VAL	B	34	4.507	60.933	31.636	1.00	27.29	B
ATOM	669	CA	VAL	B	34	3.546	61.010	32.735	1.00	25.28	B
ATOM	670	CB	VAL	B	34	3.695	59.806	33.690	1.00	26.71	B
ATOM	671	CG1	VAL	B	34	2.920	60.036	34.985	1.00	27.25	B
ATOM	672	CG2	VAL	B	34	3.176	58.565	32.997	1.00	23.84	B
ATOM	673	C	VAL	B	34	3.822	62.310	33.476	1.00	22.65	B
ATOM	674	O	VAL	B	34	2.899	63.064	33.763	1.00	21.36	B
ATOM	675	N	TRP	B	35	5.100	62.580	33.757	1.00	22.24	B
ATOM	676	CA	TRP	B	35	5.502	63.828	34.414	1.00	20.87	B
ATOM	677	CB	TRP	B	35	7.016	63.843	34.653	1.00	23.71	B
ATOM	678	CG	TRP	B	35	7.523	65.040	35.434	1.00	26.08	B
ATOM	679	CD2	TRP	B	35	7.013	65.551	36.681	1.00	25.13	B
ATOM	680	CE2	TRP	B	35	7.767	66.698	37.003	1.00	28.35	B
ATOM	681	CE3	TRP	B	35	5.985	65.143	37.547	1.00	24.83	B
ATOM	682	CD1	TRP	B	35	8.540	65.880	35.074	1.00	25.67	B
ATOM	683	NE1	TRP	B	35	8.692	66.877	36.006	1.00	27.74	B
ATOM	684	CZ2	TRP	B	35	7.532	67.455	38.165	1.00	28.38	B
ATOM	685	C23	TRP	B	35	5.749	65.889	38.699	1.00	23.47	B
ATOM	686	CH2	TRP	B	35	6.516	67.034	38.999	1.00	28.31	B
ATOM	687	C	TRP	B	35	5.121	65.039	33.564	1.00	24.26	B
ATOM	688	O	TRP	B	35	4.695	66.063	34.088	1.00	23.94	B
ATOM	689	N	GLY	B	36	5.308	64.927	32.247	1.00	25.59	B
ATOM	690	CA	GLY	B	36	4.961	66.013	31.348	1.00	23.22	B
ATOM	691	C	GLY	B	36	3.479	66.364	31.343	1.00	25.72	B
ATOM	692	O	GLY	B	36	3.138	67.539	31.352	1.00	28.94	B
ATOM	693	N	ILE	B	37	2.610	65.356	31.311	1.00	27.20	B
ATOM	694	CA	ILE	B	37	1.160	65.560	31.315	1.00	24.67	B
ATOM	695	CB	ILE	B	37	0.429	64.223	31.230	1.00	24.72	B
ATOM	696	CG2	ILE	B	37	-1.085	64.410	31.416	1.00	29.15	B
ATOM	697	CG1	ILE	B	37	0.700	63.581	29.879	1.00	22.40	B
ATOM	698	CD1	ILE	B	37	0.023	62.237	29.714	1.00	24.46	B
ATOM	699	C	ILE	B	37	0.734	66.295	32.579	1.00	25.86	B
ATOM	700	O	ILE	B	37	-0.019	67.255	32.517	1.00	25.23	B
ATOM	701	N	LYS	B	38	1.242	65.840	33.722	1.00	26.17	B
ATOM	702	CA	LYS	B	38	0.967	66.449	35.020	1.00	22.96	B
ATOM	703	CB	LYS	B	38	1.656	65.652	36.130	1.00	22.07	B
ATOM	704	CG	LYS	B	38	0.953	64.410	36.522	1.00	25.14	B
ATOM	705	CD	LYS	B	38	-0.225	64.727	37.423	1.00	28.48	B
ATOM	706	CE	LYS	B	38	-1.014	63.468	37.617	1.00	28.77	B
ATOM	707	NZ	LYS	B	38	-1.331	62.953	36.269	1.00	34.06	B
ATOM	708	C	LYS	B	38	1.458	67.877	35.102	1.00	23.87	B
ATOM	709	O	LYS	B	38	0.770	68.736	35.640	1.00	20.93	B
ATOM	710	N	GLN	B	39	2.662	68.140	34.593	1.00	26.53	B
ATOM	711	CA	GLN	B	39	3.189	69.493	34.682	1.00	30.76	B

Figure 11L

ATOM	712	CB	GLN	B	39	4.629	69.583	34.197	1.00	33.05	B
ATOM	713	CG	GLN	B	39	5.436	70.614	34.985	1.00	43.49	B
ATOM	714	CD	GLN	B	39	4.822	72.026	35.008	1.00	48.65	B
ATOM	715	OE1	GLN	B	39	4.889	72.774	34.021	1.00	51.46	B
ATOM	716	NE2	GLN	B	39	4.220	72.389	36.143	1.00	47.35	B
ATOM	717	C	GLN	B	39	2.343	70.417	33.843	1.00	31.81	B
ATOM	718	O	GLN	B	39	2.125	71.574	34.206	1.00	31.08	B
ATOM	719	N	LEU	B	40	1.897	69.904	32.703	1.00	31.01	B
ATOM	720	CA	LEU	B	40	1.065	70.671	31.807	1.00	33.41	B
ATOM	721	CB	LEU	B	40	0.872	69.886	30.517	1.00	32.63	B
ATOM	722	CG	LEU	B	40	-0.126	70.405	29.482	1.00	34.65	B
ATOM	723	CD1	LEU	B	40	0.171	71.843	29.092	1.00	35.24	B
ATOM	724	CD2	LEU	B	40	-0.058	69.495	28.281	1.00	35.90	B
ATOM	725	C	LEU	B	40	-0.289	70.943	32.469	1.00	36.85	B
ATOM	726	O	LEU	B	40	-0.874	72.010	32.314	1.00	37.81	B
ATOM	727	N	GLN	B	41	-0.768	69.964	33.215	1.00	36.13	B
ATOM	728	CA	GLN	B	41	-2.046	70.063	33.894	1.00	37.74	B
ATOM	729	CB	GLN	B	41	-2.369	68.718	34.517	1.00	41.31	B
ATOM	730	CG	GLN	B	41	-3.833	68.459	34.735	1.00	47.08	B
ATOM	731	CD	GLN	B	41	-4.070	67.139	35.420	1.00	54.09	B
ATOM	732	OE1	GLN	B	41	-3.517	66.102	35.013	1.00	55.42	B
ATOM	733	NE2	GLN	B	41	-4.908	67.154	36.461	1.00	54.90	B
ATOM	734	C	GLN	B	41	-2.039	71.148	34.974	1.00	39.95	B
ATOM	735	O	GLN	B	41	-2.988	71.925	35.089	1.00	39.23	B
ATOM	736	N	ALA	B	42	-0.972	71.194	35.767	1.00	39.05	B
ATOM	737	CA	ALA	B	42	-0.845	72.188	36.824	1.00	38.56	B
ATOM	738	CB	ALA	B	42	0.345	71.852	37.757	1.00	34.14	B
ATOM	739	C	ALA	B	42	-0.647	73.566	36.228	1.00	40.18	B
ATOM	740	O	ALA	B	42	-1.139	74.560	36.765	1.00	41.44	B
ATOM	741	N	ARG	B	43	0.078	73.634	35.118	1.00	41.82	B
ATOM	742	CA	ARG	B	43	0.340	74.910	34.476	1.00	43.71	B
ATOM	743	CB	ARG	B	43	1.242	74.713	33.260	1.00	47.26	B
ATOM	744	CG	ARG	B	43	1.703	75.997	32.592	1.00	51.08	B
ATOM	745	CD	ARG	B	43	2.582	75.677	31.401	1.00	54.95	B
ATOM	746	NE	ARG	B	43	3.778	74.947	31.813	1.00	57.04	B
ATOM	747	CZ	ARG	B	43	4.819	75.499	32.428	1.00	56.95	B
ATOM	748	NH1	ARG	B	43	4.816	76.794	32.703	1.00	55.89	B
ATOM	749	NH2	ARG	B	43	5.858	74.753	32.781	1.00	57.00	B
ATOM	750	C	ARG	B	43	-0.987	75.521	34.048	1.00	42.38	B
ATOM	751	O	ARG	B	43	-1.308	76.657	34.398	1.00	41.41	B
ATOM	752	N	ILE	B	44	-1.756	74.736	33.310	1.00	41.63	B
ATOM	753	CA	ILE	B	44	-3.059	75.143	32.810	1.00	43.24	B
ATOM	754	CB	ILE	B	44	-3.634	74.085	31.866	1.00	44.23	B
ATOM	755	CG2	ILE	B	44	-5.083	74.403	31.592	1.00	45.04	B
ATOM	756	CG1	ILE	B	44	-2.778	73.964	30.600	1.00	47.45	B
ATOM	757	CD1	ILE	B	44	-3.156	72.745	29.719	1.00	49.42	B
ATOM	758	C	ILE	B	44	-4.081	75.306	33.935	1.00	42.37	B
ATOM	759	O	ILE	B	44	-4.422	76.416	34.332	1.00	42.08	B
ATOM	760	N	LEU	B	45	-4.573	74.162	34.398	1.00	42.20	B
ATOM	761	CA	LEU	B	45	-5.564	74.042	35.450	1.00	43.16	B
ATOM	762	CB	LEU	B	45	-6.041	72.592	35.513	1.00	46.08	B
ATOM	763	CG	LEU	B	45	-6.459	72.001	34.162	1.00	47.45	B
ATOM	764	CD1	LEU	B	45	-7.011	70.594	34.357	1.00	47.51	B
ATOM	765	CD2	LEU	B	45	-7.504	72.899	33.521	1.00	48.61	B
ATOM	766	C	LEU	B	45	-5.016	74.467	36.810	1.00	42.48	B
ATOM	767	O	LEU	B	45	-5.674	75.260	37.483	1.00	45.15	B
ATOM	768	NT	LEU	B	45	-3.945	73.987	37.206	1.00	45.66	B
ATOM	769	CA	ACE	C	0	15.143	11.286	26.819	1.00	82.49	C
ATOM	770	C	ACE	C	0	14.856	12.476	27.674	1.00	82.44	C
ATOM	771	O	ACE	C	0	13.700	12.858	27.851	1.00	84.06	C

Figure 11M

ATOM	772	N	ARG	C	1	15.890	13.103	28.220	1.00	82.91	C
ATOM	773	CA	ARG	C	1	15.663	14.253	29.073	1.00	83.87	C
ATOM	774	CB	ARG	C	1	16.156	13.970	30.491	1.00	83.74	C
ATOM	775	CG	ARG	C	1	15.769	15.065	31.456	1.00	83.47	C
ATOM	776	CD	ARG	C	1	14.340	15.542	31.156	1.00	81.66	C
ATOM	777	NE	ARG	C	1	13.249	14.748	31.726	1.00	81.00	C
ATOM	778	CZ	ARG	C	1	13.069	13.434	31.597	1.00	79.16	C
ATOM	779	NH1	ARG	C	1	13.901	12.678	30.889	1.00	79.80	C
ATOM	780	NH2	ARG	C	1	12.010	12.875	32.168	1.00	79.18	C
ATOM	781	C	ARG	C	1	16.282	15.541	28.550	1.00	85.03	C
ATOM	782	O	ARG	C	1	15.975	16.644	29.016	1.00	85.10	C
ATOM	783	N	MET	C	2	17.169	15.394	27.581	1.00	85.40	C
ATOM	784	CA	MET	C	2	17.778	16.568	27.012	1.00	86.91	C
ATOM	785	CB	MET	C	2	19.063	16.215	26.290	1.00	88.20	C
ATOM	786	CG	MET	C	2	19.711	17.410	25.653	1.00	89.72	C
ATOM	787	SD	MET	C	2	21.192	16.917	24.823	1.00	94.98	C
ATOM	788	CE	MET	C	2	22.111	16.349	26.176	1.00	91.53	C
ATOM	789	C	MET	C	2	16.771	17.154	26.036	1.00	87.44	C
ATOM	790	O	MET	C	2	16.699	18.368	25.872	1.00	89.05	C
ATOM	791	N	LYS	C	3	16.001	16.278	25.391	1.00	85.66	C
ATOM	792	CA	LYS	C	3	14.973	16.712	24.444	1.00	83.09	C
ATOM	793	CB	LYS	C	3	14.033	15.551	24.107	1.00	82.50	C
ATOM	794	CG	LYS	C	3	12.921	15.895	23.122	1.00	81.54	C
ATOM	795	CD	LYS	C	3	11.926	14.746	23.005	1.00	81.93	C
ATOM	796	CE	LYS	C	3	10.866	15.022	21.952	1.00	80.79	C
ATOM	797	NZ	LYS	C	3	10.154	16.300	22.214	1.00	82.56	C
ATOM	798	C	LYS	C	3	14.177	17.809	25.128	1.00	82.12	C
ATOM	799	O	LYS	C	3	14.053	18.925	24.617	1.00	81.76	C
ATOM	800	N	GLN	C	4	13.651	17.474	26.302	1.00	80.32	C
ATOM	801	CA	GLN	C	4	12.856	18.401	27.094	1.00	78.87	C
ATOM	802	CB	GLN	C	4	12.504	17.759	28.440	1.00	79.91	C
ATOM	803	CG	GLN	C	4	12.122	16.275	28.356	1.00	80.66	C
ATOM	804	CD	GLN	C	4	11.087	15.971	27.280	1.00	81.02	C
ATOM	805	OE1	GLN	C	4	11.348	16.140	26.082	1.00	79.52	C
ATOM	806	NE2	GLN	C	4	9.907	15.516	27.701	1.00	81.57	C
ATOM	807	C	GLN	C	4	13.667	19.680	27.299	1.00	77.97	C
ATOM	808	O	GLN	C	4	13.186	20.781	27.032	1.00	78.45	C
ATOM	809	N	ILE	C	5	14.902	19.530	27.772	1.00	76.07	C
ATOM	810	CA	ILE	C	5	15.785	20.670	27.974	1.00	73.89	C
ATOM	811	CB	ILE	C	5	17.206	20.220	28.381	1.00	73.07	C
ATOM	812	CG2	ILE	C	5	18.175	21.388	28.264	1.00	71.17	C
ATOM	813	CG1	ILE	C	5	17.174	19.623	29.795	1.00	72.84	C
ATOM	814	CD1	ILE	C	5	18.518	19.113	30.285	1.00	71.39	C
ATOM	815	C	ILE	C	5	15.880	21.423	26.656	1.00	74.14	C
ATOM	816	O	ILE	C	5	15.939	22.651	26.628	1.00	73.70	C
ATOM	817	N	GLU	C	6	15.895	20.664	25.567	1.00	73.88	C
ATOM	818	CA	GLU	C	6	15.972	21.222	24.225	1.00	73.70	C
ATOM	819	CB	GLU	C	6	16.395	20.135	23.229	1.00	72.24	C
ATOM	820	CG	GLU	C	6	17.787	19.535	23.464	1.00	69.96	C
ATOM	821	CD	GLU	C	6	18.922	20.428	22.985	1.00	68.01	C
ATOM	822	OE1	GLU	C	6	19.044	21.575	23.461	1.00	65.93	C
ATOM	823	OE2	GLU	C	6	19.702	19.963	22.125	1.00	68.18	C
ATOM	824	C	GLU	C	6	14.602	21.773	23.842	1.00	74.50	C
ATOM	825	O	GLU	C	6	14.476	22.546	22.890	1.00	75.27	C
ATOM	826	N	ASP	C	7	13.577	21.372	24.587	1.00	74.82	C
ATOM	827	CA	ASP	C	7	12.218	21.838	24.327	1.00	76.17	C
ATOM	828	CB	ASP	C	7	11.195	20.742	24.644	1.00	77.40	C
ATOM	829	CG	ASP	C	7	11.408	19.488	23.818	1.00	78.45	C
ATOM	830	OD1	ASP	C	7	11.518	19.609	22.580	1.00	79.26	C
ATOM	831	OD2	ASP	C	7	11.452	18.380	24.404	1.00	79.10	C

Figure 11N

ATOM	832	C	ASP	C	7	11.906	23.079	25.160	1.00	75.92	C
ATOM	833	O	ASP	C	7	11.379	24.063	24.643	1.00	77.15	C
ATOM	834	N	LYS	C	8	12.223	23.024	26.452	1.00	74.05	C
ATOM	835	CA	LYS	C	8	11.987	24.157	27.336	1.00	71.19	C
ATOM	836	CB	LYS	C	8	12.565	23.886	28.727	1.00	72.69	C
ATOM	837	CG	LYS	C	8	11.647	24.225	29.901	1.00	72.96	C
ATOM	838	CD	LYS	C	8	10.428	23.312	29.921	1.00	75.00	C
ATOM	839	CE	LYS	C	8	9.587	23.471	31.197	1.00	76.69	C
ATOM	840	NZ	LYS	C	8	8.998	24.829	31.389	1.00	73.68	C
ATOM	841	C	LYS	C	8	12.727	25.319	26.679	1.00	69.24	C
ATOM	842	O	LYS	C	8	12.295	26.469	26.745	1.00	69.77	C
ATOM	843	N	ILE	C	9	13.855	25.013	26.046	1.00	65.63	C
ATOM	844	CA	ILE	C	9	14.609	26.053	25.362	1.00	64.27	C
ATOM	845	CB	ILE	C	9	15.950	25.511	24.812	1.00	62.88	C
ATOM	846	CG2	ILE	C	9	16.585	26.515	23.871	1.00	62.42	C
ATOM	847	CG1	ILE	C	9	16.900	25.231	25.976	1.00	64.19	C
ATOM	848	CD1	ILE	C	9	18.244	24.656	25.557	1.00	64.32	C
ATOM	849	C	ILE	C	9	13.756	26.605	24.223	1.00	63.69	C
ATOM	850	O	ILE	C	9	13.735	27.816	23.985	1.00	63.21	C
ATOM	851	N	GLU	C	10	13.036	25.712	23.543	1.00	62.89	C
ATOM	852	CA	GLU	C	10	12.163	26.092	22.429	1.00	62.21	C
ATOM	853	CB	GLU	C	10	11.419	24.865	21.886	1.00	63.68	C
ATOM	854	CG	GLU	C	10	10.451	25.180	20.751	1.00	66.12	C
ATOM	855	CD	GLU	C	10	9.688	23.961	20.251	1.00	67.29	C
ATOM	856	OE1	GLU	C	10	8.874	24.125	19.318	1.00	69.26	C
ATOM	857	OE2	GLU	C	10	9.894	22.845	20.780	1.00	68.71	C
ATOM	858	C	GLU	C	10	11.142	27.147	22.831	1.00	60.65	C
ATOM	859	O	GLU	C	10	10.991	28.157	22.147	1.00	60.16	C
ATOM	860	N	GLU	C	11	10.429	26.898	23.927	1.00	60.41	C
ATOM	861	CA	GLU	C	11	9.415	27.826	24.435	1.00	58.98	C
ATOM	862	CB	GLU	C	11	8.736	27.243	25.683	1.00	59.35	C
ATOM	863	CG	GLU	C	11	9.709	26.588	26.652	1.00	61.78	C
ATOM	864	CD	GLU	C	11	9.376	26.801	28.127	1.00	63.00	C
ATOM	865	OE1	GLU	C	11	9.329	27.972	28.563	1.00	64.82	C
ATOM	866	OE2	GLU	C	11	9.184	25.804	28.855	1.00	60.50	C
ATOM	867	C	GLU	C	11	10.021	29.186	24.772	1.00	58.03	C
ATOM	868	O	GLU	C	11	9.519	30.229	24.351	1.00	59.21	C
ATOM	869	N	ILE	C	12	11.103	29.178	25.532	1.00	56.15	C
ATOM	870	CA	ILE	C	12	11.765	30.415	25.902	1.00	56.41	C
ATOM	871	CB	ILE	C	12	13.043	30.139	26.710	1.00	55.29	C
ATOM	872	CG2	ILE	C	12	13.791	31.448	26.950	1.00	52.26	C
ATOM	873	CG1	ILE	C	12	12.680	29.404	28.008	1.00	55.06	C
ATOM	874	CD1	ILE	C	12	13.858	29.085	28.914	1.00	55.11	C
ATOM	875	C	ILE	C	12	12.132	31.239	24.671	1.00	57.76	C
ATOM	876	O	ILE	C	12	11.944	32.454	24.659	1.00	59.18	C
ATOM	877	N	GLU	C	13	12.668	30.589	23.642	1.00	60.62	C
ATOM	878	CA	GLU	C	13	13.039	31.312	22.423	1.00	62.64	C
ATOM	879	CB	GLU	C	13	13.916	30.449	21.497	1.00	66.02	C
ATOM	880	CG	GLU	C	13	13.319	29.091	21.138	1.00	70.85	C
ATOM	881	CD	GLU	C	13	14.091	28.355	20.041	1.00	73.58	C
ATOM	882	OE1	GLU	C	13	15.330	28.233	20.163	1.00	72.99	C
ATOM	883	OE2	GLU	C	13	13.456	27.887	19.064	1.00	73.78	C
ATOM	884	C	GLU	C	13	11.785	31.748	21.679	1.00	60.74	C
ATOM	885	O	GLU	C	13	11.808	32.733	20.946	1.00	61.13	C
ATOM	886	N	SER	C	14	10.695	31.010	21.864	1.00	59.71	C
ATOM	887	CA	SER	C	14	9.432	31.350	21.211	1.00	60.53	C
ATOM	888	CB	SER	C	14	8.392	30.248	21.439	1.00	59.88	C
ATOM	889	OG	SER	C	14	7.157	30.571	20.820	1.00	56.34	C
ATOM	890	C	SER	C	14	8.921	32.668	21.790	1.00	61.04	C
ATOM	891	O	SER	C	14	8.793	33.655	21.073	1.00	59.08	C

Figure 11O

ATOM	892	N	LYS	C	15	8.632	32.671	23.091	1.00	62.79	C
ATOM	893	CA	LYS	C	15	8.153	33.873	23.771	1.00	64.30	C
ATOM	894	CB	LYS	C	15	7.949	33.612	25.273	1.00	65.74	C
ATOM	895	CG	LYS	C	15	6.637	32.903	25.642	1.00	68.25	C
ATOM	896	CD	LYS	C	15	6.534	32.695	27.154	1.00	69.92	C
ATOM	897	CE	LYS	C	15	5.186	32.131	27.564	1.00	70.69	C
ATOM	898	NZ	LYS	C	15	4.078	33.079	27.241	1.00	73.69	C
ATOM	899	C	LYS	C	15	9.130	35.029	23.601	1.00	64.03	C
ATOM	900	O	LYS	C	15	8.723	36.175	23.408	1.00	64.04	C
ATOM	901	N	GLN	C	16	10.418	34.721	23.678	1.00	63.47	C
ATOM	902	CA	GLN	C	16	11.451	35.733	23.537	1.00	65.82	C
ATOM	903	CB	GLN	C	16	12.813	35.064	23.393	1.00	65.17	C
ATOM	904	CG	GLN	C	16	13.970	36.027	23.413	1.00	65.29	C
ATOM	905	CD	GLN	C	16	14.944	35.695	24.516	1.00	66.93	C
ATOM	906	OE1	GLN	C	16	15.940	36.389	24.719	1.00	68.97	C
ATOM	907	NE2	GLN	C	16	14.657	34.621	25.244	1.00	66.55	C
ATOM	908	C	GLN	C	16	11.157	36.605	22.317	1.00	67.53	C
ATOM	909	O	GLN	C	16	11.172	37.836	22.397	1.00	68.90	C
ATOM	910	N	LYS	C	17	10.886	35.952	21.193	1.00	67.63	C
ATOM	911	CA	LYS	C	17	10.566	36.648	19.954	1.00	67.83	C
ATOM	912	CB	LYS	C	17	10.355	35.627	18.833	1.00	69.39	C
ATOM	913	CG	LYS	C	17	9.747	36.199	17.556	1.00	72.05	C
ATOM	914	CD	LYS	C	17	10.657	37.203	16.835	1.00	73.47	C
ATOM	915	CE	LYS	C	17	9.946	37.784	15.613	1.00	74.71	C
ATOM	916	NZ	LYS	C	17	10.885	38.603	14.795	1.00	76.15	C
ATOM	917	C	LYS	C	17	9.306	37.492	20.123	1.00	66.64	C
ATOM	918	O	LYS	C	17	9.244	38.632	19.652	1.00	67.45	C
ATOM	919	N	LYS	C	18	8.300	36.924	20.784	1.00	64.29	C
ATOM	920	CA	LYS	C	18	7.049	37.641	21.019	1.00	63.62	C
ATOM	921	CB	LYS	C	18	5.979	36.719	21.627	1.00	64.15	C
ATOM	922	CG	LYS	C	18	5.088	36.062	20.586	1.00	66.52	C
ATOM	923	CD	LYS	C	18	3.935	35.297	21.220	1.00	68.98	C
ATOM	924	CE	LYS	C	18	4.427	34.076	21.970	1.00	70.96	C
ATOM	925	NZ	LYS	C	18	5.098	33.116	21.040	1.00	72.62	C
ATOM	926	C	LYS	C	18	7.265	38.852	21.922	1.00	61.00	C
ATOM	927	O	LYS	C	18	6.854	39.958	21.585	1.00	61.84	C
ATOM	928	N	ILE	C	19	7.904	38.653	23.067	1.00	56.58	C
ATOM	929	CA	ILE	C	19	8.179	39.765	23.961	1.00	53.92	C
ATOM	930	CB	ILE	C	19	9.101	39.329	25.119	1.00	52.10	C
ATOM	931	CG2	ILE	C	19	9.719	40.545	25.799	1.00	51.95	C
ATOM	932	CG1	ILE	C	19	8.304	38.463	26.095	1.00	51.65	C
ATOM	933	CD1	ILE	C	19	9.103	37.908	27.247	1.00	50.93	C
ATOM	934	C	ILE	C	19	8.833	40.893	23.165	1.00	53.24	C
ATOM	935	O	ILE	C	19	8.604	42.069	23.438	1.00	52.35	C
ATOM	936	N	GLU	C	20	9.642	40.534	22.173	1.00	53.82	C
ATOM	937	CA	GLU	C	20	10.294	41.536	21.338	1.00	54.86	C
ATOM	938	CB	GLU	C	20	11.393	40.910	20.472	1.00	55.74	C
ATOM	939	CG	GLU	C	20	12.554	40.318	21.251	1.00	56.50	C
ATOM	940	CD	GLU	C	20	13.683	39.851	20.352	1.00	56.98	C
ATOM	941	OE1	GLU	C	20	13.473	38.918	19.543	1.00	56.87	C
ATOM	942	OE2	GLU	C	20	14.786	40.427	20.453	1.00	58.79	C
ATOM	943	C	GLU	C	20	9.245	42.188	20.437	1.00	55.80	C
ATOM	944	O	GLU	C	20	9.311	43.382	20.166	1.00	55.44	C
ATOM	945	N	ASN	C	21	8.289	41.389	19.972	1.00	55.46	C
ATOM	946	CA	ASN	C	21	7.223	41.899	19.118	1.00	57.62	C
ATOM	947	CB	ASN	C	21	6.392	40.754	18.530	1.00	59.92	C
ATOM	948	CG	ASN	C	21	7.060	40.101	17.325	1.00	63.29	C
ATOM	949	OD1	ASN	C	21	6.574	39.092	16.806	1.00	62.67	C
ATOM	950	ND2	ASN	C	21	8.169	40.684	16.866	1.00	61.87	C
ATOM	951	C	ASN	C	21	6.307	42.829	19.891	1.00	58.25	C

Figure 11P

ATOM	952	O	ASN	C	21	5.649	43.697	19.309	1.00	59.75	C
ATOM	953	N	GLU	C	22	6.255	42.645	21.206	1.00	56.32	C
ATOM	954	CA	GLU	C	22	5.411	43.489	22.030	1.00	53.64	C
ATOM	955	CB	GLU	C	22	5.014	42.756	23.313	1.00	55.42	C
ATOM	956	CG	GLU	C	22	3.786	43.357	23.967	1.00	60.12	C
ATOM	957	CD	GLU	C	22	2.506	43.082	23.188	1.00	61.82	C
ATOM	958	OE1	GLU	C	22	2.559	43.024	21.942	1.00	62.49	C
ATOM	959	OE2	GLU	C	22	1.435	42.954	23.825	1.00	63.39	C
ATOM	960	C	GLU	C	22	6.158	44.791	22.344	1.00	50.89	C
ATOM	961	O	GLU	C	22	5.573	45.873	22.282	1.00	49.72	C
ATOM	962	N	ILE	C	23	7.448	44.691	22.665	1.00	47.08	C
ATOM	963	CA	ILE	C	23	8.259	45.876	22.948	1.00	46.40	C
ATOM	964	CB	ILE	C	23	9.752	45.504	23.290	1.00	47.53	C
ATOM	965	CG2	ILE	C	23	10.707	46.653	22.910	1.00	44.86	C
ATOM	966	CG1	ILE	C	23	9.898	45.178	24.783	1.00	45.28	C
ATOM	967	CD1	ILE	C	23	9.101	44.004	25.256	1.00	45.91	C
ATOM	968	C	ILE	C	23	8.222	46.771	21.717	1.00	46.76	C
ATOM	969	O	ILE	C	23	8.317	47.999	21.822	1.00	46.87	C
ATOM	970	N	ALA	C	24	8.071	46.137	20.556	1.00	47.50	C
ATOM	971	CA	ALA	C	24	8.002	46.828	19.271	1.00	46.10	C
ATOM	972	CB	ALA	C	24	8.112	45.809	18.126	1.00	44.51	C
ATOM	973	C	ALA	C	24	6.706	47.644	19.137	1.00	45.09	C
ATOM	974	O	ALA	C	24	6.741	48.810	18.752	1.00	43.05	C
ATOM	975	N	ARG	C	25	5.566	47.034	19.445	1.00	43.64	C
ATOM	976	CA	ARG	C	25	4.301	47.753	19.346	1.00	45.79	C
ATOM	977	CB	ARG	C	25	3.115	46.807	19.581	1.00	44.07	C
ATOM	978	CG	ARG	C	25	3.045	45.680	18.564	1.00	48.16	C
ATOM	979	CD	ARG	C	25	1.677	44.986	18.458	1.00	50.13	C
ATOM	980	NE	ARG	C	25	1.216	44.299	19.664	1.00	54.12	C
ATOM	981	CZ	ARG	C	25	0.665	44.888	20.725	1.00	58.36	C
ATOM	982	NH1	ARG	C	25	0.475	46.206	20.756	1.00	59.26	C
ATOM	983	NH2	ARG	C	25	0.268	44.148	21.755	1.00	59.83	C
ATOM	984	C	ARG	C	25	4.257	48.908	20.345	1.00	47.24	C
ATOM	985	O	ARG	C	25	3.941	50.038	19.978	1.00	50.68	C
ATOM	986	N	ILE	C	26	4.584	48.617	21.601	1.00	47.54	C
ATOM	987	CA	ILE	C	26	4.591	49.608	22.673	1.00	44.40	C
ATOM	988	CB	ILE	C	26	5.042	48.959	24.001	1.00	43.91	C
ATOM	989	CG2	ILE	C	26	5.259	50.026	25.071	1.00	45.47	C
ATOM	990	CG1	ILE	C	26	4.010	47.930	24.450	1.00	42.59	C
ATOM	991	CD1	ILE	C	26	4.445	47.138	25.663	1.00	40.19	C
ATOM	992	C	ILE	C	26	5.532	50.766	22.379	1.00	44.58	C
ATOM	993	O	ILE	C	26	5.193	51.935	22.564	1.00	42.04	C
ATOM	994	N	LYS	C	27	6.721	50.422	21.919	1.00	46.75	C
ATOM	995	CA	LYS	C	27	7.754	51.394	21.619	1.00	51.78	C
ATOM	996	CB	LYS	C	27	8.915	50.674	20.951	1.00	54.23	C
ATOM	997	CG	LYS	C	27	10.184	51.465	20.863	1.00	57.21	C
ATOM	998	CD	LYS	C	27	11.313	50.479	20.644	1.00	60.99	C
ATOM	999	CE	LYS	C	27	12.660	51.064	21.014	1.00	62.83	C
ATOM	1000	NZ	LYS	C	27	13.750	50.060	20.828	1.00	64.49	C
ATOM	1001	C	LYS	C	27	7.299	52.556	20.750	1.00	52.44	C
ATOM	1002	O	LYS	C	27	7.334	53.710	21.165	1.00	54.11	C
ATOM	1003	N	LYS	C	28	6.877	52.239	19.538	1.00	53.88	C
ATOM	1004	CA	LYS	C	28	6.435	53.250	18.599	1.00	55.29	C
ATOM	1005	CB	LYS	C	28	6.169	52.582	17.249	1.00	57.59	C
ATOM	1006	CG	LYS	C	28	7.390	51.841	16.717	1.00	59.15	C
ATOM	1007	CD	LYS	C	28	7.041	50.830	15.635	1.00	62.19	C
ATOM	1008	CE	LYS	C	28	8.292	50.088	15.158	1.00	63.12	C
ATOM	1009	NZ	LYS	C	28	9.029	49.411	16.282	1.00	65.69	C
ATOM	1010	C	LYS	C	28	5.187	53.931	19.122	1.00	55.14	C
ATOM	1011	O	LYS	C	28	5.052	55.147	19.030	1.00	57.43	C

Figure 11Q

ATOM	1012	N	LEU	C	29	4.275	53.138	19.671	1.00	52.27	C
ATOM	1013	CA	LEU	C	29	3.025	53.649	20.214	1.00	51.04	C
ATOM	1014	CB	LEU	C	29	2.281	52.485	20.855	1.00	51.13	C
ATOM	1015	CG	LEU	C	29	0.776	52.493	21.051	1.00	50.66	C
ATOM	1016	CD1	LEU	C	29	0.051	52.868	19.755	1.00	51.59	C
ATOM	1017	CD2	LEU	C	29	0.389	51.100	21.491	1.00	50.29	C
ATOM	1018	C	LEU	C	29	3.347	54.739	21.245	1.00	50.83	C
ATOM	1019	O	LEU	C	29	2.739	55.805	21.269	1.00	53.58	C
ATOM	1020	N	LEU	C	30	4.327	54.457	22.089	1.00	50.52	C
ATOM	1021	CA	LEU	C	30	4.767	55.397	23.100	1.00	48.88	C
ATOM	1022	CB	LEU	C	30	5.813	54.730	23.997	1.00	48.03	C
ATOM	1023	CG	LEU	C	30	6.485	55.530	25.113	1.00	47.31	C
ATOM	1024	CD1	LEU	C	30	5.447	56.172	26.033	1.00	45.24	C
ATOM	1025	CD2	LEU	C	30	7.398	54.575	25.889	1.00	48.28	C
ATOM	1026	C	LEU	C	30	5.374	56.587	22.379	1.00	48.83	C
ATOM	1027	O	LEU	C	30	5.020	57.736	22.642	1.00	48.40	C
ATOM	1028	N	GLN	C	31	6.298	56.289	21.470	1.00	49.93	C
ATOM	1029	CA	GLN	C	31	6.983	57.304	20.670	1.00	52.00	C
ATOM	1030	CB	GLN	C	31	7.822	56.609	19.590	1.00	55.56	C
ATOM	1031	CG	GLN	C	31	8.628	57.513	18.645	1.00	61.26	C
ATOM	1032	CD	GLN	C	31	9.768	58.241	19.333	1.00	64.58	C
ATOM	1033	OE1	GLN	C	31	10.233	57.818	20.391	1.00	68.00	C
ATOM	1034	NE2	GLN	C	31	10.249	59.318	18.715	1.00	64.37	C
ATOM	1035	C	GLN	C	31	5.947	58.225	20.009	1.00	49.56	C
ATOM	1036	O	GLN	C	31	6.192	59.415	19.814	1.00	45.68	C
ATOM	1037	N	LEU	C	32	4.793	57.657	19.675	1.00	47.64	C
ATOM	1038	CA	LEU	C	32	3.723	58.401	19.034	1.00	48.95	C
ATOM	1039	CB	LEU	C	32	2.689	57.433	18.461	1.00	50.72	C
ATOM	1040	CG	LEU	C	32	1.602	57.935	17.502	1.00	51.93	C
ATOM	1041	CD1	LEU	C	32	2.209	58.293	16.154	1.00	50.26	C
ATOM	1042	CD2	LEU	C	32	0.554	56.840	17.313	1.00	51.55	C
ATOM	1043	C	LEU	C	32	3.070	59.295	20.077	1.00	49.32	C
ATOM	1044	O	LEU	C	32	3.040	60.519	19.929	1.00	50.01	C
ATOM	1045	N	THR	C	33	2.545	58.659	21.125	1.00	48.74	C
ATOM	1046	CA	THR	C	33	1.878	59.324	22.246	1.00	43.86	C
ATOM	1047	CB	THR	C	33	1.643	58.329	23.400	1.00	46.04	C
ATOM	1048	OG1	THR	C	33	0.707	57.332	22.977	1.00	47.18	C
ATOM	1049	CG2	THR	C	33	1.121	59.039	24.639	1.00	42.89	C
ATOM	1050	C	THR	C	33	2.683	60.494	22.771	1.00	41.04	C
ATOM	1051	O	THR	C	33	2.132	61.537	23.122	1.00	39.26	C
ATOM	1052	N	VAL	C	34	3.992	60.303	22.843	1.00	38.83	C
ATOM	1053	CA	VAL	C	34	4.886	61.346	23.301	1.00	36.90	C
ATOM	1054	CB	VAL	C	34	6.329	60.825	23.377	1.00	33.71	C
ATOM	1055	CG1	VAL	C	34	7.270	61.907	23.904	1.00	29.40	C
ATOM	1056	CG2	VAL	C	34	6.366	59.590	24.251	1.00	31.78	C
ATOM	1057	C	VAL	C	34	4.795	62.437	22.254	1.00	38.65	C
ATOM	1058	O	VAL	C	34	4.489	63.595	22.556	1.00	39.38	C
ATOM	1059	N	TRP	C	35	5.049	62.038	21.010	1.00	42.18	C
ATOM	1060	CA	TRP	C	35	5.002	62.937	19.868	1.00	40.00	C
ATOM	1061	CB	TRP	C	35	4.991	62.134	18.563	1.00	40.06	C
ATOM	1062	CG	TRP	C	35	4.848	63.020	17.399	1.00	36.56	C
ATOM	1063	CD2	TRP	C	35	3.696	63.161	16.561	1.00	36.91	C
ATOM	1064	CE2	TRP	C	35	3.968	64.212	15.673	1.00	41.20	C
ATOM	1065	CE3	TRP	C	35	2.457	62.505	16.503	1.00	40.31	C
ATOM	1066	CD1	TRP	C	35	5.748	63.944	16.974	1.00	35.30	C
ATOM	1067	NE1	TRP	C	35	5.228	64.673	15.945	1.00	39.45	C
ATOM	1068	CZ2	TRP	C	35	3.037	64.643	14.704	1.00	38.75	C
ATOM	1069	CZ3	TRP	C	35	1.528	62.934	15.541	1.00	39.54	C
ATOM	1070	CH2	TRP	C	35	1.827	63.984	14.651	1.00	41.30	C
ATOM	1071	C	TRP	C	35	3.764	63.833	19.901	1.00	39.80	C

Figure 11R

ATOM	1072	O	TRP	C	35	3.868	65.052	19.769	1.00	38.39	C
ATOM	1073	N	GLY	C	36	2.601	63.210	20.059	1.00	36.88	C
ATOM	1074	CA	GLY	C	36	1.356	63.957	20.103	1.00	38.94	C
ATOM	1075	C	GLY	C	36	1.315	64.973	21.226	1.00	38.45	C
ATOM	1076	O	GLY	C	36	0.931	66.114	21.001	1.00	37.76	C
ATOM	1077	N	ILE	C	37	1.700	64.557	22.435	1.00	40.86	C
ATOM	1078	CA	ILE	C	37	1.724	65.442	23.604	1.00	36.66	C
ATOM	1079	CB	ILE	C	37	2.352	64.755	24.857	1.00	36.83	C
ATOM	1080	CG2	ILE	C	37	2.489	65.766	26.005	1.00	27.32	C
ATOM	1081	CG1	ILE	C	37	1.512	63.548	25.275	1.00	37.14	C
ATOM	1082	CD1	ILE	C	37	2.066	62.794	26.501	1.00	35.85	C
ATOM	1083	C	ILE	C	37	2.587	66.655	23.284	1.00	38.37	C
ATOM	1084	O	ILE	C	37	2.187	67.788	23.529	1.00	37.68	C
ATOM	1085	N	LYS	C	38	3.775	66.399	22.740	1.00	40.28	C
ATOM	1086	CA	LYS	C	38	4.717	67.456	22.381	1.00	42.51	C
ATOM	1087	CB	LYS	C	38	5.927	66.868	21.639	1.00	46.36	C
ATOM	1088	CG	LYS	C	38	7.109	67.829	21.391	1.00	52.00	C
ATOM	1089	CD	LYS	C	38	8.125	67.162	20.433	1.00	56.10	C
ATOM	1090	CE	LYS	C	38	9.365	68.008	20.096	1.00	56.61	C
ATOM	1091	NZ	LYS	C	38	10.340	68.155	21.222	1.00	59.57	C
ATOM	1092	C	LYS	C	38	3.995	68.445	21.483	1.00	42.06	C
ATOM	1093	O	LYS	C	38	4.351	69.628	21.428	1.00	41.76	C
ATOM	1094	N	GLN	C	39	2.977	67.966	20.774	1.00	39.73	C
ATOM	1095	CA	GLN	C	39	2.232	68.862	19.908	1.00	40.05	C
ATOM	1096	CB	GLN	C	39	1.499	68.100	18.778	1.00	41.27	C
ATOM	1097	CG	GLN	C	39	2.385	67.148	17.928	1.00	42.44	C
ATOM	1098	CD	GLN	C	39	3.681	67.786	17.465	1.00	42.00	C
ATOM	1099	OE1	GLN	C	39	3.678	68.822	16.813	1.00	44.81	C
ATOM	1100	NE2	GLN	C	39	4.802	67.163	17.802	1.00	46.04	C
ATOM	1101	C	GLN	C	39	1.241	69.638	20.781	1.00	36.22	C
ATOM	1102	O	GLN	C	39	1.344	70.845	20.885	1.00	34.78	C
ATOM	1103	N	LEU	C	40	0.285	68.950	21.398	1.00	34.58	C
ATOM	1104	CA	LEU	C	40	-0.696	69.625	22.268	1.00	36.22	C
ATOM	1105	CB	LEU	C	40	-1.465	68.595	23.096	1.00	34.67	C
ATOM	1106	CG	LEU	C	40	-2.365	69.192	24.186	1.00	34.61	C
ATOM	1107	CD1	LEU	C	40	-3.392	70.142	23.510	1.00	34.28	C
ATOM	1108	CD2	LEU	C	40	-3.057	68.084	24.972	1.00	30.45	C
ATOM	1109	C	LEU	C	40	-0.029	70.630	23.226	1.00	36.51	C
ATOM	1110	O	LEU	C	40	-0.494	71.755	23.419	1.00	36.17	C
ATOM	1111	N	GLN	C	41	1.068	70.220	23.832	1.00	36.56	C
ATOM	1112	CA	GLN	C	41	1.764	71.106	24.751	1.00	38.77	C
ATOM	1113	CB	GLN	C	41	2.883	70.310	25.433	1.00	38.66	C
ATOM	1114	CG	GLN	C	41	3.606	70.994	26.582	1.00	46.41	C
ATOM	1115	CD	GLN	C	41	4.245	69.979	27.529	1.00	50.25	C
ATOM	1116	OE1	GLN	C	41	4.898	69.028	27.091	1.00	53.94	C
ATOM	1117	NE2	GLN	C	41	4.063	70.180	28.831	1.00	52.04	C
ATOM	1118	C	GLN	C	41	2.291	72.336	23.998	1.00	37.58	C
ATOM	1119	O	GLN	C	41	2.190	73.466	24.486	1.00	38.73	C
ATOM	1120	N	ALA	C	42	2.627	72.128	22.795	1.00	36.75	C
ATOM	1121	CA	ALA	C	42	3.365	73.249	22.014	1.00	36.93	C
ATOM	1122	CB	ALA	C	42	4.084	72.717	20.779	1.00	32.48	C
ATOM	1123	C	ALA	C	42	2.241	74.209	21.600	1.00	35.85	C
ATOM	1124	O	ALA	C	42	2.407	75.427	21.602	1.00	34.18	C
ATOM	1125	N	ARG	C	43	1.101	73.629	21.249	1.00	32.51	C
ATOM	1126	CA	ARG	C	43	-0.072	74.365	20.829	1.00	34.59	C
ATOM	1127	CB	ARG	C	43	-1.152	73.357	20.524	1.00	34.80	C
ATOM	1128	CG	ARG	C	43	-2.467	73.891	20.060	1.00	36.54	C
ATOM	1129	CD	ARG	C	43	-3.310	72.667	19.769	1.00	37.93	C
ATOM	1130	NE	ARG	C	43	-4.631	72.945	19.236	1.00	40.51	C
ATOM	1131	CZ	ARG	C	43	-5.481	71.985	18.901	1.00	42.74	C

Figure 11S

ATOM	1132	NH1	ARG	C	43	-5.127	70.717	19.051	1.00	41.40	C
ATOM	1133	NH2	ARG	C	43	-6.676	72.288	18.421	1.00	44.00	C
ATOM	1134	C	ARG	C	43	-0.568	75.347	21.883	1.00	37.96	C
ATOM	1135	O	ARG	C	43	-1.049	76.425	21.558	1.00	36.78	C
ATOM	1136	N	ILE	C	44	-0.434	74.971	23.151	1.00	41.66	C
ATOM	1137	CA	ILE	C	44	-0.901	75.799	24.250	1.00	43.04	C
ATOM	1138	CB	ILE	C	44	-1.403	74.891	25.390	1.00	45.88	C
ATOM	1139	CG2	ILE	C	44	-1.802	75.717	26.594	1.00	46.21	C
ATOM	1140	CG1	ILE	C	44	-2.572	74.041	24.876	1.00	46.16	C
ATOM	1141	CD1	ILE	C	44	-2.926	72.877	25.786	1.00	50.31	C
ATOM	1142	C	ILE	C	44	0.109	76.802	24.807	1.00	41.15	C
ATOM	1143	O	ILE	C	44	-0.235	77.961	25.047	1.00	40.03	C
ATOM	1144	N	LEU	C	45	1.345	76.350	25.005	1.00	40.33	C
ATOM	1145	CA	LEU	C	45	2.401	77.184	25.579	1.00	39.81	C
ATOM	1146	CB	LEU	C	45	3.357	76.322	26.422	1.00	40.22	C
ATOM	1147	CG	LEU	C	45	2.889	75.608	27.694	1.00	40.80	C
ATOM	1148	CD1	LEU	C	45	1.733	74.714	27.364	1.00	42.51	C
ATOM	1149	CD2	LEU	C	45	4.029	74.789	28.299	1.00	39.44	C
ATOM	1150	C	LEU	C	45	3.215	77.953	24.540	1.00	38.95	C
ATOM	1151	O	LEU	C	45	3.071	77.689	23.327	1.00	39.83	C
ATOM	1152	NT	LEU	C	45	4.014	78.810	24.964	1.00	39.47	C
ATOM	1153	OH2	TIP	W	2	8.280	62.369	27.138	1.00	38.82	W
ATOM	1154	OH2	TIP	W	3	28.782	24.001	17.582	1.00	78.47	W
ATOM	1155	OH2	TIP	W	4	0.492	62.209	33.896	1.00	50.43	W
ATOM	1156	OH2	TIP	W	5	6.020	70.609	23.199	1.00	45.29	W
ATOM	1157	OH2	TIP	W	6	1.993	78.695	31.896	1.00	37.25	W
ATOM	1158	OH2	TIP	W	7	20.294	18.975	19.485	1.00	49.56	W
ATOM	1159	OH2	TIP	W	8	18.592	15.442	35.405	1.00	34.86	W
ATOM	1160	OH2	TIP	W	9	-5.907	64.337	32.524	1.00	31.24	W
ATOM	1161	OH2	TIP	W	10	11.567	18.853	30.945	1.00	47.94	W
ATOM	1162	OH2	TIP	W	11	-9.321	65.456	23.794	1.00	46.60	W
ATOM	1163	OH2	TIP	W	12	-2.842	65.953	28.078	1.00	59.15	W
ATOM	1164	OH2	TIP	W	13	-1.409	77.305	18.859	1.00	37.51	W
ATOM	1165	OH2	TIP	W	14	-5.597	64.224	37.408	1.00	39.02	W
ATOM	1166	OH2	TIP	W	15	-5.079	75.908	18.460	1.00	48.65	W
ATOM	1167	OH2	TIP	W	16	12.444	58.431	21.920	1.00	62.97	W
ATOM	1168	OH2	TIP	W	17	-12.927	70.555	24.520	1.00	61.81	W
ATOM	1169	OH2	TIP	W	18	14.897	23.356	34.046	1.00	40.13	W
ATOM	1170	OH2	TIP	W	19	3.154	40.721	28.964	1.00	29.89	W
ATOM	1171	OH2	TIP	W	20	4.290	81.951	24.440	1.00	44.83	W
ATOM	1172	OH2	TIP	W	21	26.490	23.104	32.265	1.00	62.67	W
ATOM	1173	OH2	TIP	W	22	13.085	59.162	33.622	1.00	54.53	W
ATOM	1174	OH2	TIP	W	23	-0.166	45.626	35.200	1.00	56.34	W
ATOM	1175	OH2	TIP	W	24	-10.278	62.692	33.867	1.00	64.05	W
ATOM	1176	OH2	TIP	W	25	22.697	10.892	29.710	1.00	100.00	W
ATOM	1177	OH2	TIP	W	26	4.281	39.194	26.136	1.00	62.29	W
ATOM	1178	OH2	TIP	W	27	22.833	20.843	19.882	1.00	59.57	W
ATOM	1179	OH2	TIP	W	28	-10.030	74.838	23.517	1.00	53.18	W
ATOM	1180	OH2	TIP	W	29	1.246	80.456	24.973	1.00	36.18	W
ATOM	1181	OH2	TIP	W	30	-3.034	76.181	17.506	1.00	50.44	W
ATOM	1182	OH2	TIP	W	31	1.424	49.275	18.155	1.00	44.03	W
ATOM	1183	OH2	TIP	W	32	6.269	64.921	23.710	1.00	31.68	W
ATOM	1184	OH2	TIP	W	33	27.134	28.497	40.798	1.00	60.31	W
ATOM	1185	OH2	TIP	W	34	24.326	28.221	41.517	1.00	85.52	W
ATOM	1186	OH2	TIP	W	35	24.492	26.009	31.850	1.00	68.20	W
ATOM	1187	OH2	TIP	W	36	17.270	23.540	41.621	1.00	45.61	W
ATOM	1188	OH2	TIP	W	37	17.175	27.169	41.299	1.00	57.26	W
ATOM	1189	OH2	TIP	W	38	17.133	30.154	42.769	1.00	94.65	W
ATOM	1190	OH2	TIP	W	39	23.961	29.473	38.207	1.00	73.43	W
ATOM	1191	OH2	TIP	W	40	26.646	30.299	35.030	1.00	86.46	W

Figure 11T

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ATOM   1192  OH2 TIP W  41      21.799  33.921  37.475  1.00 98.23      W
ATOM   1193  OH2 TIP W  42      12.296  24.508  37.800  1.00 73.10      W
ATOM   1194  OH2 TIP W  43      10.910  28.524  40.599  1.00 65.23      W
ATOM   1195  OH2 TIP W  44       8.726  30.065  36.214  1.00 62.46      W
ATOM   1196  OH2 TIP W  45      20.748  34.061  34.804  1.00 62.12      W
ATOM   1197  OH2 TIP W  46       7.462  29.159  29.170  1.00 88.23      W
ATOM   1198  OH2 TIP W  47       7.466  31.280  33.124  1.00 56.10      W
ATOM   1199  OH2 TIP W  48       6.666  26.619  36.241  1.00 52.76      W
ATOM   1200  OH2 TIP W  49       3.823  27.148  35.557  1.00 92.76      W
ATOM   1201  OH2 TIP W  50       7.608  28.183  32.367  1.00 83.54      W
ATOM   1202  OH2 TIP W  51      10.064  35.767  38.975  1.00 68.12      W
ATOM   1203  OH2 TIP W  52      14.649  36.973  38.236  1.00 73.09      W
ATOM   1204  OH2 TIP W  53      16.799  36.406  39.778  1.00 48.69      W
ATOM   1205  OH2 TIP W  54      15.456  39.954  39.598  1.00 48.97      W
ATOM   1206  OH2 TIP W  55       8.442  41.891  37.753  1.00 57.63      W
ATOM   1207  OH2 TIP W  56       9.926  44.040  39.986  1.00 80.20      W
ATOM   1208  OH2 TIP W  57       3.713  35.630  32.034  1.00 65.94      W
ATOM   1209  OH2 TIP W  58       4.004  32.569  30.481  1.00 98.02      W
ATOM   1210  OH2 TIP W  59      13.514  45.594  36.374  1.00 45.92      W
ATOM   1211  OH2 TIP W  60      12.274  44.358  32.693  1.00 69.72      W
ATOM   1212  OH2 TIP W  61      -1.770  41.459  30.288  1.00 86.62      W
ATOM   1213  OH2 TIP W  62      -0.747  39.619  34.003  1.00 85.57      W
ATOM   1214  OH2 TIP W  63       2.370  42.056  36.997  1.00 63.26      W
ATOM   1215  OH2 TIP W  64       7.646  47.813  26.559  1.00 86.77      W
ATOM   1216  OH2 TIP W  65      -1.942  50.096  25.818  1.00 33.47      W
ATOM   1217  OH2 TIP W  66      -0.455  48.262  24.057  1.00 48.49      W
ATOM   1218  OH2 TIP W  67      -1.850  44.976  32.352  1.00 46.88      W
ATOM   1219  OH2 TIP W  68      -4.779  47.469  30.587  1.00 53.38      W
ATOM   1220  OH2 TIP W  69      -8.800  47.417  33.155  1.00 55.34      W
ATOM   1221  OH2 TIP W  70      -7.762  51.374  35.608  1.00 72.46      W
ATOM   1222  OH2 TIP W  71       5.493  50.307  35.418  1.00 63.93      W
ATOM   1223  OH2 TIP W  72      -2.293  60.557  33.176  1.00 58.13      W
ATOM   1224  OH2 TIP W  73      -3.891  59.956  22.859  1.00 42.99      W
ATOM   1225  OH2 TIP W  74      -2.324  52.365  23.808  1.00 68.12      W
ATOM   1226  OH2 TIP W  75      -4.610  53.603  23.534  1.00 99.86      W
ATOM   1227  OH2 TIP W  76      -5.369  51.351  24.806  1.00 66.59      W
ATOM   1228  OH2 TIP W  77      -9.158  53.927  27.711  1.00 59.38      W
ATOM   1229  OH2 TIP W  78      -6.839  60.379  22.155  1.00 48.43      W
ATOM   1230  OH2 TIP W  79      -7.811  55.209  31.835  1.00 63.25      W
ATOM   1231  OH2 TIP W  80      -8.988  55.740  34.680  1.00 48.03      W
ATOM   1232  OH2 TIP W  81     -14.358  62.793  31.478  1.00 77.34      W
ATOM   1233  OH2 TIP W  82     -14.884  67.194  30.264  1.00100.00      W
ATOM   1234  OH2 TIP W  83     -13.964  62.903  27.850  1.00 61.59      W
ATOM   1235  OH2 TIP W  84     -16.467  64.338  27.598  1.00 62.99      W
ATOM   1236  OH2 TIP W  85     -14.165  71.419  31.235  1.00 58.55      W
ATOM   1237  OH2 TIP W  86     -12.150  75.052  20.683  1.00 54.74      W
ATOM   1238  OH2 TIP W  87     -15.348  66.527  23.972  1.00 86.65      W
ATOM   1239  OH2 TIP W  88      23.657  18.784  16.110  1.00 46.11      W
ATOM   1240  OH2 TIP W  89      21.774  13.448  17.383  1.00 55.62      W
ATOM   1241  OH2 TIP W  90      28.955  20.801  18.398  1.00 47.29      W
ATOM   1242  OH2 TIP W  91      19.043  22.428  18.931  1.00 70.31      W
ATOM   1243  OH2 TIP W  92      32.348  21.741  32.055  1.00 80.85      W
ATOM   1244  OH2 TIP W  93      31.544  26.386  31.293  1.00 80.53      W
ATOM   1245  OH2 TIP W  94      30.484  31.504  24.099  1.00 51.19      W
ATOM   1246  OH2 TIP W  95      28.981  30.812  18.458  1.00 98.45      W
ATOM   1247  OH2 TIP W  96      25.233  35.680  28.569  1.00 53.47      W
ATOM   1248  OH2 TIP W  97      25.740  37.432  31.266  1.00 96.40      W
ATOM   1249  OH2 TIP W  98      18.343  27.853  17.008  1.00 87.39      W
ATOM   1250  OH2 TIP W  99      26.162  40.002  24.887  1.00 63.29      W
ATOM   1251  OH2 TIP W 100      18.896  37.649  32.149  1.00 75.85      W
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Figure 11U

ATOM	1252	OH2	TIP	W	101	20.897	31.301	18.264	1.00	88.40	W
ATOM	1253	OH2	TIP	W	102	19.191	42.582	21.453	1.00	55.18	W
ATOM	1254	OH2	TIP	W	103	23.958	41.188	26.907	1.00	78.30	W
ATOM	1255	OH2	TIP	W	104	18.433	46.716	22.932	1.00	54.59	W
ATOM	1256	OH2	TIP	W	105	22.353	48.547	25.042	1.00	59.94	W
ATOM	1257	OH2	TIP	W	106	21.797	41.049	34.496	1.00	78.60	W
ATOM	1258	OH2	TIP	W	107	21.437	46.210	33.535	1.00	75.53	W
ATOM	1259	OH2	TIP	W	108	14.907	43.959	21.380	1.00	54.65	W
ATOM	1260	OH2	TIP	W	109	15.635	42.456	19.119	1.00	58.03	W
ATOM	1261	OH2	TIP	W	110	19.533	44.310	33.666	1.00	80.58	W
ATOM	1262	OH2	TIP	W	111	18.747	50.736	29.399	1.00	60.97	W
ATOM	1263	OH2	TIP	W	112	21.131	52.757	28.680	1.00	55.70	W
ATOM	1264	OH2	TIP	W	113	17.303	55.311	38.133	1.00	72.59	W
ATOM	1265	OH2	TIP	W	114	18.939	58.215	28.845	1.00	79.75	W
ATOM	1266	OH2	TIP	W	115	14.666	59.680	28.964	1.00	50.64	W
ATOM	1267	OH2	TIP	W	116	17.408	62.649	28.523	1.00	74.43	W
ATOM	1268	OH2	TIP	W	117	12.106	61.533	23.810	1.00	89.64	W
ATOM	1269	OH2	TIP	W	118	10.138	60.131	37.626	1.00	89.60	W
ATOM	1270	OH2	TIP	W	119	14.125	60.999	36.831	1.00	78.03	W
ATOM	1271	OH2	TIP	W	120	6.987	65.584	27.400	1.00	63.28	W
ATOM	1272	OH2	TIP	W	121	8.699	65.761	30.950	1.00	64.96	W
ATOM	1273	OH2	TIP	W	122	11.912	66.582	33.458	1.00	45.24	W
ATOM	1274	OH2	TIP	W	123	7.712	69.520	31.053	1.00	89.81	W
ATOM	1275	OH2	TIP	W	124	0.300	66.328	28.053	1.00	83.63	W
ATOM	1276	OH2	TIP	W	125	18.739	12.093	36.575	1.00	68.16	W
ATOM	1277	OH2	TIP	W	126	8.341	17.901	23.874	1.00	69.12	W
ATOM	1278	OH2	TIP	W	127	6.665	20.667	30.766	1.00	79.31	W
ATOM	1279	OH2	TIP	W	128	13.178	21.216	32.239	1.00	55.97	W
ATOM	1280	OH2	TIP	W	129	7.700	21.187	21.255	1.00	66.56	W
ATOM	1281	OH2	TIP	W	130	17.038	26.024	19.828	1.00	40.17	W
ATOM	1282	OH2	TIP	W	131	9.682	31.384	16.376	1.00	77.12	W
ATOM	1283	OH2	TIP	W	132	11.568	29.117	15.187	1.00	59.43	W
ATOM	1284	OH2	TIP	W	133	2.602	30.287	27.387	1.00	64.52	W
ATOM	1285	OH2	TIP	W	134	10.743	41.812	16.813	1.00	84.35	W
ATOM	1286	OH2	TIP	W	135	13.070	38.706	12.664	1.00	61.24	W
ATOM	1287	OH2	TIP	W	136	9.262	44.518	14.939	1.00	51.92	W
ATOM	1288	OH2	TIP	W	137	12.139	53.137	17.554	1.00	56.22	W
ATOM	1289	OH2	TIP	W	138	14.403	57.453	15.838	1.00	66.72	W
ATOM	1290	OH2	TIP	W	139	11.017	71.423	23.035	1.00	71.76	W
ATOM	1291	OH2	TIP	W	140	10.451	75.718	24.795	1.00	58.85	W
ATOM	1292	OH2	TIP	W	141	11.223	65.048	21.172	1.00	84.46	W
ATOM	1293	OH2	TIP	W	142	8.196	70.691	21.387	1.00	66.14	W
ATOM	1294	OH2	TIP	W	143	3.381	51.168	17.717	1.00	51.91	W
ATOM	1295	OH2	TIP	W	144	13.735	48.059	19.325	1.00	73.18	W
ATOM	1296	OH2	TIP	W	145	2.524	42.027	17.393	1.00	80.66	W
ATOM	1297	OH2	TIP	W	146	2.024	39.150	18.549	1.00	74.07	W
ATOM	1298	OH2	TIP	W	147	0.486	41.584	19.991	1.00	97.41	W
ATOM	1299	OH2	TIP	W	148	0.060	40.945	24.577	1.00	78.10	W
ATOM	1300	OH2	TIP	W	149	14.261	36.624	16.034	1.00	71.76	W
ATOM	1301	OH2	TIP	W	150	17.041	33.288	18.134	1.00	55.41	W
ATOM	1302	OH2	TIP	W	151	12.012	53.850	23.650	1.00	34.32	W
ATOM	1303	OH2	TIP	W	152	0.421	41.869	28.444	1.00	53.88	W
ATOM	1304	CL-1	CL	I	1	13.184	36.734	27.569	1.00	62.34	I
END											

Figure 11V